United States
Department of
Agriculture

Agricultural
Research
Service

Technical
Bulletin
Number 1661

Analytical Solutions of the One-Dimensional Convective-Dispersive Solute Transport Equation

ABSTRACT

M. Th. van Genuchten and W. J. Alves. 1982. Analytical Solutions of the One-Dimensional Convective-Dispersive Solute Transport Equation. U.S. Department of Agriculture, Technical Bulletin No. 1661, 151 p.

This compendium lists available mathematical models and associated computer programs for solution of the one-dimensional convective-dispersive solute transport equation. The governing transport equations include terms accounting for convection, diffusion and dispersion, and linear equilibrium adsorption. In some cases, the effects of zero-order production and first-order decay have also been taken into account. Numerous analytical solutions of the general transport equation have been published, both in well-known and widely distributed journals and in lesser known reports or conference proceedings. This study brings together the most common of these solutions in one publication.

Some of the listed solutions have been published previously. Many others, however, were not available and have been derived to make the list of solutions more complete. User-oriented FORTRAN IV computer programs of several analytical solutions and one numerical solution are given in an appendix. A list of Laplace transforms used to derive the analytical solutions is provided also.

Keywords: Salt movement, solute transport models, analytical solutions, equilibrium adsorption, degradation, convective-dispersive transport, Laplace transforms, boundary conditions, miscible displacement.

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Issued June 1982

Analytical Solutions of the One-Dimensional Convective-Dispersive Solute Transport Equation

By M. Th. van Genuchten and W. J. Alves [1]

1. INTRODUCTION

The rate at which a chemical constituent moves through soil is determined by several transport mechanisms. These mechanisms often act simultaneously on the chemical and may include such processes as convection, diffusion and dispersion, linear equilibrium adsorption, and zero-order or first-order production and decay. Because of the many mechanisms affecting solute transport, a complete set of analytical solutions should be available, not only for predicting actual solute transport in the field but also for analyzing the transport mechanisms themselves, for example, in conjuction with column displacement experiments.

This publication lists mathematical models and several computer programs for solution of the one-dimensional convective-dispersive solute transport equation. Numerous analytical solutions of this equation have been published in recent years, both in well-known and widely distributed scientific journals and in lesser known reports and conference proceedings. This publication brings together the most common of these solutions in one publication.

Several of the listed solutions have been published previously. Many others, however, are new and were derived to make the list of solutions more complete. User-oriented FORTRAN IV computer programs of several analytical solutions are given in an appendix. All programs were successfully tested on an IBM 370/155 computer. Furthermore, results of each program were compared with results based on a numerical solution of the governing transport equation; this was done to check the programming accuracy of each solution. Card-deck copies of all computer programs, including those listed in appendix B, are available upon request.

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2. THE GOVERNING TRANSPORT EQUATION

The partial differential equation describing one-dimensional chemical transport under transient fluid flow conditions is taken as

$$\frac{\partial}{\partial x}\left(\theta D \frac{\partial c}{\partial x} - qc\right) - \frac{\partial}{\partial t}(\theta c + \rho s) = \mu_w \theta c + \mu_s \rho s - \gamma_w \theta - \gamma_s \rho \qquad [1]$$

where c is the solution concentration (ML^{-3}), s is the adsorbed concentration (MM^{-1}), θ is the volumetric moisture content (L^3L^{-3}), D is the dispersion coefficient (L^2T^{-1}), q is the volumetric flux (LT^{-1}), ρ is the porous medium bulk density (ML^{-3}), x is the distance (L), and t is time (T). The coefficients μ_w and μ_s are rate constants for first-order decay in the liquid and solid phases of the soil (T^{-1}). The coefficients γ_w and γ_s represent similar rate constants for zero-order production in the two soil phases ($ML^{-3}T^{-1}$ and T^{-1}, respectively).

The solution of [1] requires an expression relating the adsorbed concentration (s) with the solution concentration (c). Several types of models for adsorption or ion exchange are available for this purpose, such as equilibrium and non-equilibrium models. In this study only single-ion equilibrium transport is considered, and the general adsorption isotherm is described by a linear (or linearized) equation of the form

$$s = k\,c \qquad [2]$$

where k is an empirical distribution constant ($M^{-1}L^3$). Substitution of [2] into [1] gives

$$\frac{\partial}{\partial x}\left(\theta D \frac{\partial c}{\partial x} - qc\right) - \frac{\partial(\theta R c)}{\partial t} = \mu\theta c - \gamma\theta \qquad [3]$$

where the retardation factor R is given by

$$R = 1 + \rho k/\theta, \qquad [4]$$

and with the new rate coefficients μ and γ given by

$$\mu = \mu_w + \mu_s \rho k/\theta \qquad [5]$$

$$\gamma = \gamma_w + \gamma_s \rho/\theta. \qquad [6]$$

When the volumetric moisture content and the volumetric flux remain constant in time and space (steady-state flow), the transport equation reduces to

$$D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} - R \frac{\partial c}{\partial t} = \mu c - \gamma \qquad [7]$$

where v $(=q/\theta)$ is the interstitial or pore-water velocity. Equation [7], or its appropriate simplifications, has found widespread application in soil science, chemical and environmental engineering, and water resources. Some of the known applications include the movement of ammonium or nitrate in soils (Gardner *1965*, Reddy et al. *1976*, Misra and Mishra *1977*),[2] pesticide movement (Kay and Elrick *1967*, van Genuchten and Wierenga *1974*), the transport of radioactive waste materials (Arnett et al. *1976*, Duguid and Reeves *1977*), the fixation of certain iron and zinc chelates (Lahav and Hochberg *1975*), and the precipitation and dissolution of gypsum (Kemper et al. *1975*, Glas et al. *1979*, Keisling et al. *1978*) or other salts (Melamed et al. *1977*). Transport equations similar to [7] have also been applied to saltwater intrusion problems in coastal aquifers (Shamir and Harleman *1966*), to thermal and contaminant pollution of rivers and lakes (Cleary *1971*, Thomann *1973*, Baron and Wajc *1976* , DiToro *1974*), and to convective heat transfer problems in general (Lykov and Mikhailov *1961*, Carslaw and Jaeger(*1959*).

3. INITIAL AND BOUNDARY CONDITIONS

This compendium gives analytical solutions of [7] subject to various initial and boundary conditions. The general initial condition is

$$c(x,0) = f(x) \qquad (t = 0) \qquad [8]$$

where $f(x)$ can take on several forms: a constant value with distance, an exponentially increasing or decreasing function with x, or a steady-state type distribution for production or decay. Two different boundary conditions can be applied at $x = 0$: a first- or concentration-type boundary condition of the form

$$c(0,t) = g(t) \qquad (x = 0) \qquad [9a]$$

or a third- or flux-type boundary condition of the form

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[2]The year in italic, when it follows the author's name, refers to Literature Cited, p. 98.

$$-D \frac{\partial c}{\partial x} + vc = v\, g(t) \qquad (x = 0) \qquad [9b]$$

where g(t) also can take on several distributions, such as a constant value in time (continuous feed solution), a pulse-type distribution, or an exponentially increasing or decreasing function with time. Note that [9b] does lead to conservation of mass inside a soil column, whereas [9a] may lead to mass balance errors when applied to displacement experiments in which the tracer solution is injected at a prescribed rate. These errors can become significant for relatively large values of the ratio (D/v).

For the lower boundary, the following condition can be applied

$$\frac{\partial c}{\partial x} (\infty, t) = 0. \qquad [10a]$$

This condition assumes the presence of a semi-infinite soil column. When analytical solutions based on this boundary condition are used to calculate effluent curves from finite columns, some errors may be introduced. An alternative boundary condition, one that is used frequently for displacement studies, is that of a zero concentration gradient at the lower end of the column:

$$\frac{\partial c}{\partial x} (L, t) = 0 \qquad [10b]$$

where L is the column length. This condition, which leads to a continuous concentration distribution at x=L, has been discussed extensively in the literature (Wehner and Wilhelm *1956*, Pearson *1959*, van Genuchten and Wierenga *1974*, Bear *1979*). In our opinion, no clear evidence exists that [10b] leads to a better description of the physical processes at and around x=L than [10a]. Moreover, boundary condition [9b] does lead to a discontinuous concentration distribution at the column entrance (x=0) and, as such, seems to contradict the requirement of having to have a continuous distribution at x=L.

In this study, we present analytical solutions for both lower boundary conditions ([10a] and [10b]). Because of the relatively small influence of the imposed mathematical boundary conditions, the analytical solutions for a semi-infinite system should provide close approximations for analytical solutions that are applicable to a physically well-defined finite system, especially for laboratory soil columns that are not too short.

Boundary condition [10a] cannot be applied to Eq. [7] for the particular case when $\mu = 0$ and $\gamma > 0$. The lower boundary condition for a semi-infinite system that is subject to zero-order production only (no first-order decay) is

$$\frac{\partial c}{\partial x}(\infty, t) = \text{finite}. \qquad [10c]$$

Table 1 summarizes the various mathematical models for which analytical solutions are given in the next section. The governing equations and associated initial and boundary conditions are grouped into three categories: Category A, where the governing transport equation has no production and decay terms ($\gamma = \mu = 0$); category B, for zero-order production only ($\gamma \neq 0$; $\mu = 0$); and category C, for simultaneous zero-order production and first-order decay ($\gamma \neq 0$, $\mu \neq 0$). No special category is given for those models in which the transport equation has only a first-order decay term ($\gamma = 0$; $\mu \neq 0$). The analytical solutions for these cases follow immediately from those of category C by simply putting $\gamma = 0$ in the various expressions. A similar reduction from category C to category B, by assuming $\mu = 0$, is mathematically not possible because of divisions by zero.

Table 1.--Summary of mathematical models for which analytical solutions are given

Governing Equation

$$R\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x}$$

Case	Initial condition f(x)[1]	Upper boundary condition: Type[2]	Upper boundary condition: g(t)[3]	Lower boundary condition[4]
A1	C_i	1	C_o (pulse)[5]	Semi-infinite.
A2	--do--	3	--do--	--do--
A3	--do--	1	--do--	Finite.
A4	--do--	3	--do--	--do--
A5	$\begin{cases} C_1 & (0 \leq x \leq x_1) \\ C_2 & (x > x_1) \end{cases}$	1	--do--	Semi-infinite.
A6	--do--	3	--do--	--do--

See footnotes at end of table.

Table 1.--Summary of mathematical models for which analytical solutions are given--Continued

Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x}$$

Case	Initial condition f(x)[1]	Upper boundary condition Type[2]	Upper boundary condition g(t)[3]	Lower boundary condition[4]
A7	$C_1 + C_2 e^{-\alpha x}$	1	C_o (pulse)[5]	--do--
A8	--do--	3	--do--	--do--
A9	C_i	1	$C_a + C_b e^{-\lambda t}$	Semi-infinite.
A10	--do--	3	--do--	--do--
A11	--do--	1	--do--	Finite.
A12	--do--	3	--do--	--do--

Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} + \gamma$$

Case	Initial condition f(x)[1]	Upper boundary condition Type[2]	Upper boundary condition g(t)[3]	Lower boundary condition[4]
B1	NA[6]	1	C_o	Semi-inifite.
B2	--do--	3	--do--	--do--
B3	--do--	1	--do--	Finite.
B4	--do--	3	--do--	--do--
B5	C_i	1	C_o (pulse)	Semi-infinite.
B6	--do--	3	--do--	--do--
B7	--do--	1	--do--	Finite.
B8	--do--	3	--do--	--do--
B9	ST-ST[7]	1	--do--	Semi-infinite.
B10	--do--	3	--do--	--do--
B11	--do--	1	--do--	Finite.
B12	--do--	3	--do--	--do--
B13	C_i	1	$C_a + C_b e^{-\lambda t}$	Semi-infinite.
B14	--do--	3	--do--	--do--
B15	--do--	1	--do--	Finite.
B16	--do--	3	--do--	--do--

See footnotes at end of table.

Table 1.--Summary of mathematical models for which analytical solutions are given--Continued

Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} - \mu c + \gamma$$

Case	Initial Condition $f(x)$[1]	Upper boundary condition: Type[2]	Upper boundary condition: $g(t)$[3]	Lower boundary condition[4]
C1	NA[6]	1	C_o	Semi-infinite.
C2	--do--	3	--do--	--do--
C3	--do--	1	--do--	Finite.
C4	--do--	3	--do--	--do--
C5	C_i	1	C_o (pulse)[5]	Semi-infinite.
C6	--do--	3	--do--	--do--
C7	--do--	1	--do--	Finite.
C8	--do--	3	--do--	--do--
C9	ST-ST[7]	1	--do--	Semi-infinite.
C10	--do--	3	--do--	--do--
C11	--do--	1	--do--	Finite.
C12	--do--	3	--do--	--do--
C13	C_i	1	$C_a + C_b e^{-\lambda t}$	Semi-infinite.
C14	--do--	3	--do--	--do--
C15	--do--	1	--do--	Finite.
C16	--do--	3	--do--	--do--

[1] $f(x)$ in equation [8].
[2] '1' for a first-type boundary condition (equation [9a]); '3' for a third-type boundary condition (equation [9b]).
[3] $g(t)$ in Eq. [9a] or [9b].
[4] Equation [10a] or [10c] for a semi-infinite system; equation [10b] for a finite system.
[5] Indicates a pulse-type application:

$$g(t) = \begin{cases} C_o & (0 < t \leq t_o) \\ 0 & (t > t_o) \end{cases}$$

[6] Not applicable; steady-state solution.
[7] Steady-state type initial distribution.

4. LIST OF ANALYTICAL SOLUTIONS

This section presents analytical solutions of [7], with or without the two rate terms, subject to the initial and boundary conditions summarized in table 1. Several of the listed solutions have been published previously. Others, however, were not available and have been derived to make the list as complete as possible. Laplace transform techniques were generally used to derive those new solutions that are applicable to a semi-infinite system (boundary conditions [10a] or [10c]). Appendix A lists useful Laplace transforms, many of them unpublished.

Inspection of the various analytical solutions shows that all solutions for a finite system, that is, those based on boundary condition [10b], are in the form of infinite series. These series solutions converge slowly for relatively large values of the dimensionless group

$$P = vL/D \qquad [11]$$

where P is often referred to as the column Peclet number. Using Laplace transform techniques in a similar way as shown by Brenner (*1962*), approximate solutions were derived that provide accurate answers for the larger P-values. The suggested range of application of the approximate solutions is

$$\frac{vL}{D} > 5 + 40\,\frac{vt}{RL} \qquad (P > 5 + 40\ T/R) \qquad [12a]$$

or

$$\frac{vL}{D} > 100 \qquad (P > 100) \qquad [12b]$$

whichever condition is met first. The dimensionless variable T in [12a], called the number of pore volumes when used in conjunction with column displacement studies, is given by

$$T = vt/L. \qquad [13]$$

Conditions [12a] and [12b] were obtained empirically by comparing numerous results based on series and approximate solutions. When the conditions are satisfied, an accuracy of at least four significant places will be obtained with the approximate solutions. When condition [12a] or [12b] is not satisfied, we recommend that the series solutions be used. In that case, only about 4 to 10 terms of the series are needed to assure a similar accuracy of four significant digits.

A. Solutions for No Production or Decay

A1. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x}$$

Initial and Boundary Conditions

$$c(x,0) = C_i$$

$$c(0,t) = \begin{cases} C_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(\infty,t) = 0$$

Analytical Solution (Lapidus and Amundson *1952*, Ogata and Banks *1961*)

$$c(x,t) = \begin{cases} C_i + (C_o - C_i)\, A(x,t) & 0 < t \leq t_o \\ C_i + (C_o - C_i)\, A(x,t) - C_o\, A(x,t-t_o) & t > t_o \end{cases}$$

where

$$A(x,t) = \frac{1}{2} \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \frac{1}{2} \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

A2. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x}$$

Initial and Boundary Conditions

$$c(x,0) = C_i$$

$$\left(-D \frac{\partial c}{\partial x} + vc\right)\Big|_{x=0} = \begin{cases} vC_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(\infty,t) = 0$$

Analytical Solution (Mason and Weaver *1924*, Lindstrom et al. *1967*, Gershon and Nir *1969*).

$$c(x,t) = \begin{cases} C_i + (C_o - C_i)\, A(x,t) & 0 < t \leq t_o \\ C_i + (C_o - C_i)\, A(x,t) - C_o\, A(x,t-t_o) & t > t_o \end{cases}$$

where

$$A(x,t) = \frac{1}{2}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \left(\frac{v^2 t}{\pi DR}\right)^{1/2} \exp\left[-\frac{(Rx - vt)^2}{4DRt}\right]$$

$$- \frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right) \exp(vx/D)\,\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

A3. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x}$$

Initial and Boundary Conditions

$$c(x,0) = C_i$$

$$c(0,t) = \begin{cases} C_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(L,t) = 0$$

Analytical Solution (Cleary and Adrian *1973*).

$$c(x,t) = \begin{cases} C_i + (C_o - C_i)\, A(x,t) & 0 < t \leq t_o \\ C_i + (C_o - C_i)\, A(x,t) - C_o\, A(x,t-t_o) & t > t_o \end{cases}$$

where

$$A(x,t) = 1 - \sum_{m=1}^{\infty} \frac{2\beta_m \sin(\frac{\beta_m x}{L}) \exp[\frac{vx}{2D} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}]}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{vL}{2D}]}$$

and where the eigenvalues β_m are the positive roots of the equation

$$\beta_m \cot(\beta_m) + \frac{vL}{2D} = 0$$

Approximate Solution

$$A(x,t) = \frac{1}{2}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \frac{1}{2}\exp(vx/D)\,\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{1}{2}\left[2 + \frac{v(2L - x)}{D} + \frac{v^2t}{DR}\right]\exp(vL/D)\,\mathrm{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$- \left(\frac{v^2t}{\pi DR}\right)^{1/2}\exp\left[\frac{vL}{D} - \frac{R}{4Dt}\left(2L-x + \frac{vt}{R}\right)^2\right]$$

A4. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x}$$

Initial and Boundary Conditions

$$c(x,0) = C_i$$

$$\left(-D \frac{\partial c}{\partial x} + vc\right)\Bigg|_{x=0} = \begin{cases} vC_o & 0 < t \leqslant t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(L,t) = 0$$

Analytical Solution (Brenner *1962*, see also Bastian and Lapidus *1956*).

$$c(x,t) = \begin{cases} C_i + (C_o - C_i)\, A(x,t) & 0 < t \leqslant t_o \\ C_i + (C_o - C_i)\, A(x,t) - C_o\, A(x,t-t_o) & t > t_o \end{cases}$$

where

$A(x,t) =$

$$1 - \sum_{m-1}^{\infty} \frac{\frac{2vL}{D}\, \beta_m \left[\beta_m \cos\left(\frac{\beta_m x}{L}\right) + \frac{vL}{2D} \sin\left(\frac{\beta_m x}{L}\right)\right] \exp\left[\frac{vx}{2D} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}\right]}{\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2 + \frac{vL}{D}\right]\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2\right]}$$

and where the eigenvalues β_m are the positive roots of

$$\beta_m \cot(\beta_m) - \frac{\beta_m^2 D}{vL} + \frac{vL}{4D} = 0$$

Approximate Solution (Brenner *1962*)

$$A(x,t) = \frac{1}{2}\,\text{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \left(\frac{v^2 t}{\pi DR}\right)^{1/2} \exp\left[-\frac{(Rx - vt)^2}{4DRt}\right]$$

$$- \frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right) \exp(vx/D)\,\text{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$+ \left(\frac{4v^2 t}{\pi DR}\right)^{1/2} \left[1 + \frac{v}{4D}\left(2L-x + \frac{vt}{R}\right)\right] \exp\left[\frac{vL}{D} - \frac{R}{4Dt}\left(2L-x + \frac{vt}{R}\right)^2\right]$$

$$- \frac{v}{D}\left[2L-x + \frac{3vt}{2R} + \frac{v}{4D}\left(2L-x + \frac{vt}{R}\right)^2\right] \exp(vL/D)\,\text{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

A5. Governing Equation $R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x}$

Initial and Boundary Conditions

$$c(x,0) = \begin{cases} C_1 & 0 \leq x < x_1 \\ C_2 & x \geq x_1 \end{cases}$$

$$c(0,t) = \begin{cases} C_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x} (\infty,t) = 0$$

Analytical Solution

$$c(x,t) =$$

$$\begin{cases} C_2 + (C_1 - C_2)\, A(x,t) + (C_o - C_1)\, B(x,t) & 0 < t \leq t_o \\ C_2 + (C_1 - C_2)\, A(x,t) + (C_o - C_1)\, B(x,t) - C_o\, B(x,t-t_o) & t > t_o \end{cases}$$

where

$$A(x,t) = \frac{1}{2} \operatorname{erfc}\left[\frac{R(x-x_1) - vt}{2(DRt)^{1/2}}\right] + \frac{1}{2} \exp(vx/D) \operatorname{erfc}\left[\frac{R(x+x_1) + vt}{2(DRt)^{1/2}}\right]$$

$$B(x,t) = \frac{1}{2} \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \frac{1}{2} \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

A6. Governing Equation $R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x}$

Initial and Boundary Conditions

$$c(x,0) = \begin{cases} C_1 & 0 \leqslant x < x_1 \\ C_2 & x \geqslant x_1 \end{cases}$$

$$\left(-D \frac{\partial c}{\partial x} + vc\right)\Big|_{x=0} = \begin{cases} vC_o & 0 < t \leqslant t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(\infty,t) = 0$$

Analytical Solution [see also Jost (*1952*, p. 50) and Lindstrom and Boersma (*1971*)]

$$c(x,t) =$$

$$\begin{cases} C_2 + (C_1 - C_2)\, A(x,t) + (C_o - C_1)\, B(x,t) & 0 < t \leqslant t_o \\ C_2 + (C_1 - C_2)\, A(x,t) + (C_o - C_1)\, B(x,t) - C_o\, B(x,t-t_o) & t > t_o \end{cases}$$

where

$$A(x,t) = \frac{1}{2} \operatorname{erfc}\left[\frac{R(x-x_1)-vt}{2(DRt)^{1/2}}\right] + \left(\frac{v^2 t}{\pi DR}\right)^{1/2} \exp\left[\frac{vx}{D} - \frac{R}{4Dt}\left(x+x_1+\frac{vt}{R}\right)^2\right]$$

$$- \frac{1}{2}\left[1 + \frac{v(x+x_1)}{D} + \frac{v^2 t}{DR}\right] \exp(vx/D) \operatorname{erfc}\left[\frac{R(x+x_1)+vt}{2(DRt)^{1/2}}\right]$$

$$B(x,t) = \frac{1}{2} \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \left(\frac{v^2 t}{\pi DR}\right)^{1/2} \exp\left[-\frac{(Rx-vt)^2}{4DRt}\right]$$

$$- \frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right) \exp(vx/D) \operatorname{erfc}\left[\frac{Rx+vt}{2(DRt)^{1/2}}\right]$$

A7. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x}$$

Initial and Boundary Conditions

$$c(x,0) = C_1 + C_2 e^{-\alpha x}$$

$$c(0,t) = \begin{cases} C_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(\infty,t) = 0$$

Analytical Solution

$$c(x,t) =$$

$$\begin{cases} C_1 + (C_o - C_1)\, A(x,t) + C_2\, B(x,t) & 0 < t \leq t_o \\ C_1 + (C_o - C_1)\, A(x,t) + C_2\, B(x,t) - C_o\, A(x,t-t_o) & t > t_o \end{cases}$$

where

$$A(x,t) = \frac{1}{2}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \frac{1}{2}\exp(vx/D)\,\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$B(x,t) = \frac{1}{2}\exp\left(\frac{\alpha^2 Dt}{R} + \frac{\alpha vt}{R} - \alpha x\right)\left\{2 - \mathrm{erfc}\left[\frac{Rx - (v+2\alpha D)t}{2(DRt)^{1/2}}\right]\right.$$

$$\left. - \exp\left(\frac{vx}{D} + 2\alpha x\right)\mathrm{erfc}\left[\frac{Rx + (v+2\alpha D)t}{2(DRt)^{1/2}}\right]\right\}$$

A8. Governing Equation $R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x}$

Initial and Boundary Conditions

$$c(x,0) = C_1 + C_2 e^{-\alpha x}$$

$$\left(-D \frac{\partial c}{\partial x} + vc\right)\Big|_{x=0} = \begin{cases} vC_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(\infty,t) = 0$$

Analytical Solution

$$c(x,t) =$$

$$\begin{cases} C_1 + (C_o - C_1)\, A(x,t) + C_2\, B(x,t) & 0 < t \leq t_o \\ C_1 + (C_o - C_1)\, A(x,t) + C_2\, B(x,t) - C_o\, A(x,t-t_o) & t > t_o \end{cases}$$

where

$$A(x,t) = \frac{1}{2}\, \text{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \left(\frac{v^2 t}{\pi DR}\right)^{1/2} \exp\left[-\frac{(Rx - vt)^2}{4DRt}\right]$$

$$- \frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right) \exp(vx/D)\, \text{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$B(x,t) = \exp\left(\frac{\alpha^2 Dt}{R} + \frac{\alpha vt}{R} - \alpha x\right) \left\{ 1 - \frac{1}{2}\, \text{erfc}\left[\frac{Rx - (v+2\alpha D)t}{2(DRt)^{1/2}}\right] \right.$$

$$\left. + \frac{1}{2}\left(1 + \frac{v}{\alpha D}\right) \exp\left(\frac{vx}{D} + 2\alpha x\right) \text{erfc}\left[\frac{Rx + (v+2\alpha D)t}{2(DRt)^{1/2}}\right] \right\}$$

$$- \frac{v}{2\alpha D} \exp(vx/D)\, \text{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

A9. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x}$$

Initial and Boundary Conditions

$$c(x,0) = C_i$$

$$c(0,t) = C_a + C_b e^{-\lambda t}$$

$$\frac{\partial c}{\partial x}(\infty,t) = 0$$

Analytical Solution [see Marino (*1974a*) for two special cases]

$$c(x,t) = C_i + (C_a - C_i)\, A(x,t) + C_b\, B(x,t)$$

where

$$A(x,t) = \frac{1}{2} \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \frac{1}{2} \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$B(x,t) = e^{-\lambda t} \left\{ \frac{1}{2} \exp\left[\frac{(v-y)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - yt}{2(DRt)^{1/2}}\right] + \frac{1}{2} \exp\left[\frac{(v+y)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + yt}{2(DRt)^{1/2}}\right] \right\}$$

and

$$y = v \left(1 - \frac{4\lambda DR}{v^2}\right)^{1/2}$$

A10. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x}$$

Initial and Boundary Conditions

$$c(x,0) = C_i$$

$$\left(-D \frac{\partial c}{\partial x} + vc\right)\Big|_{x=0} = v(C_a + C_b e^{-\lambda t})$$

$$\frac{\partial c}{\partial x}(\infty,t) = 0$$

Analytical Solution

$$c(x,t) = C_i + (C_a - C_i)\, A(x,t) + C_b\, B(x,t)$$

where

$$A(x,t) = \frac{1}{2} \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \left(\frac{v^2 t}{\pi DR}\right)^{1/2} \exp\left[-\frac{(Rx - vt)^2}{4DRt}\right]$$

$$- \frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right) \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$B(x,t) = e^{-\lambda t}\left\{\frac{v}{(v+y)} \exp\left[\frac{(v-y)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - yt}{2(DRt)^{1/2}}\right]\right.$$

$$\left. + \frac{v}{(v-y)} \exp\left[\frac{(v+y)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + yt}{2(DRt)^{1/2}}\right]\right\}$$

$$- \frac{v^2}{2\lambda DR} \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

and

$$y = v\left(1 - \frac{4\lambda DR}{v^2}\right)^{1/2}$$

A11. Governing Equation $R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x}$

Initial and Boundary Conditions

$$c(x,0) = C_i$$

$$c(0,t) = C_a + C_b \, e^{-\lambda t}$$

$$\frac{\partial c}{\partial x}(L,t) = 0$$

Analytical Solution

$$c(x,t) = C_i + (C_a - C_i) \, A(x,t) + C_b \, B(x,t)$$

where

$$A(x,t) = 1 - \sum_{m=1}^{\infty} E(\beta_m,x) \exp\left[\frac{vx}{2D} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}\right]$$

$$B(x,t) = e^{-\lambda t} \, [B_1(x,t) - B_2(x,t)]$$

$$B_1(x,t) = 1 + \sum_{m=1}^{\infty} \frac{E(\beta_m,x) \frac{\lambda L^2 R}{D} \exp(\frac{vx}{2D})}{[\beta_m^2 + (\frac{vL}{2D})^2 - \frac{\lambda L^2 R}{D}]}$$

$$B_2(x,t) = \sum_{m=1}^{\infty} \frac{E(\beta_m,x) \, [\beta_m^2 + (\frac{vL}{2D})^2] \exp[\frac{vx}{2D} + \lambda t - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}]}{[\beta_m^2 + (\frac{vL}{2D})^2 - \frac{\lambda L^2 R}{D}]}$$

and

$$E(\beta_m,x) = \frac{2\beta_m \sin(\frac{\beta_m x}{L})}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{vL}{2D}]}$$

The eigenvalues β_m are the positive roots of

$$\beta_m \cot(\beta_m) + \frac{vL}{2D} = 0$$

The term $B_1(x)$ converges much slower than the other terms in the series solution. This term, however, can be expressed in an alternative form that is much easier to evaluate:

$$B_1(x) = \frac{\exp[\frac{(v-y)x}{2D}] + (\frac{y-v}{y+v}) \exp[\frac{(y+v)x - 2vL}{2D}]}{[1 + (\frac{y-v}{y+v}) \exp(-yL/D)]}$$

where

$$y = v \left(1 - \frac{4\lambda DR}{v^2}\right)^{1/2}$$

<u>Approximate Solution</u>

$$A(x,t) = \frac{1}{2} \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \frac{1}{2} \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{1}{2} \left[2 + \frac{v(2L-x)}{D} + \frac{v^2 t}{DR}\right] \exp(vL/D) \operatorname{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$- \left(\frac{v^2 t}{\pi DR}\right)^{1/2} \exp\left[\frac{vL}{D} - \frac{R}{4Dt}\left(2L-x + \frac{vt}{R}\right)^2\right]$$

$$B(x,t) = e^{-\lambda t} B_3(x,t)/B_4(x)$$

where

$$B_3(x,t) = \frac{1}{2} \exp[\frac{(v-y)x}{2D}] \operatorname{erfc}\left[\frac{Rx - yt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{1}{2} \exp[\frac{(v+y)x}{2D}] \operatorname{erfc}\left[\frac{Rx + yt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{(y-v)}{2(y+v)} \exp[\frac{(v+y)x - 2yL}{2D}] \operatorname{erfc}\left[\frac{R(2L-x) - yt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{(y+v)}{2(y-v)} \exp[\frac{(v-y)x + 2yL}{2D}] \text{ erfc}\left[\frac{R(2L-x) + yt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v^2}{2\lambda DR} \exp(\frac{vL}{D} + \lambda t) \text{ erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$B_4(x) = 1 + (\frac{y-v}{y+v}) \exp(-yL/D)$$

and

$$y = v \left(1 - \frac{4\lambda DR}{v^2}\right)^{1/2}$$

A12. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x}$$

<u>Initial and Boundary Conditions</u>

$$c(x,0) = C_i$$

$$\left(-D \frac{\partial c}{\partial x} + vc\right)\Bigg|_{x=0} = v(C_a + C_b\, e^{-\lambda t})$$

$$\frac{\partial c}{\partial x}(L,t) = 0$$

<u>Analytical Solution</u>

$$c(x,t) = C_i + (C_a - C_i)\, A(x,t) + C_b\, B(x,t)$$

where

$$A(x,t) = 1 - \sum_{m=1}^{\infty} E(\beta_m,x)\, \exp\left[\frac{vx}{2D} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}\right]$$

$$B(x,t) = e^{-\lambda t}\,[B_1(x) - B_2(x,t)]$$

$$B_1(x) = 1 + \sum_{m=1}^{\infty} \frac{E(\beta_m,x)\, \frac{\lambda L^2 R}{D}\, \exp\left(\frac{vx}{2D}\right)}{\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2 - \frac{\lambda L^2 R}{D}\right]}$$

$$B_2(x,t) = \sum_{m=1}^{\infty} \frac{E(\beta_m,x)\, \left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2\right] \exp\left[\frac{vx}{2D} + \lambda t - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}\right]}{\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2 - \frac{\lambda L^2 R}{D}\right]}$$

and

$$E(\beta_m,x) = \frac{\frac{2vL}{D}\, \beta_m \left[\beta_m \cos\left(\frac{\beta_m x}{L}\right) + \frac{vL}{2D} \sin\left(\frac{\beta_m x}{L}\right)\right]}{\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2 + \frac{vL}{D}\right]\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2\right]}$$

The eigenvalues β_m are the positive roots of

$$\beta_m \cot(\beta_m) - \frac{\beta_m^2 D}{vL} + \frac{vL}{4D} = 0$$

The term $B_1(x)$ converges much slower than the other terms in the series solution. This term, however, can be expressed in an alternative form that is much easier to evaluate:

$$B_1(x) = \frac{\exp[\frac{(v-y)x}{2D}] + (\frac{y-v}{y+v}) \exp[\frac{(v+y)x - 2yL}{2D}]}{[\frac{y+v}{2v} - \frac{(y-v)^2}{2v(y+v)} \exp(-yL/D)]}$$

where

$$y = v\ (1 - \frac{4\lambda D}{v^2})^{1/2}$$

<u>Approximate Solution</u>

$$A(x,t) = \frac{1}{2}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + (\frac{v^2 t}{\pi DR})^{1/2} \exp[-\frac{(Rx - vt)^2}{4DRt}]$$

$$- \frac{1}{2}\ (1 + \frac{vx}{D} + \frac{v^2 t}{DR}) \exp(vx/D)\ \mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$+ (\frac{4v^2 t}{\pi DR})^{1/2}\ [1 + \frac{v}{4D}(2L-x + \frac{vt}{R})]\ \exp[\frac{vL}{D} - \frac{R}{4Dt}(2L-x + \frac{vt}{R})^2\ ]$$

$$- \frac{v}{D}\ [2L-x + \frac{3vt}{2R} + \frac{v}{4D}(2L-x + \frac{vt}{R})^2\ ]\ \exp(vL/D)\ \mathrm{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$B(x,t) = e^{-\lambda t}\ B_3(x,t)/B_4(x)$$

where

$$B_3(x,t) = (\frac{v}{v+y}) \exp[\frac{(v-y)x}{2D}]\ \mathrm{erfc}\left[\frac{Rx - yt}{2(DRt)^{1/2}}\right]$$

$$+ \left(\frac{v}{v-y}\right) \exp\left[\frac{(v+y)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + yt}{2(DRt)^{1/2}}\right]$$

$$- \frac{v^2}{2\lambda DR} \exp\left(\frac{vx}{D} + \lambda t\right) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$- \frac{v^2}{2\lambda DR} \left[\frac{v(2L-x)}{D} + \frac{v^2 t}{DR} + 3 - \frac{v^2}{\lambda DR}\right] \exp\left(\frac{vL}{D} + \lambda t\right) \operatorname{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v^3}{\lambda DR} \left(\frac{t}{\pi DR}\right)^{1/2} \exp\left[\frac{vL}{D} + \lambda t - \frac{R}{4Dt}\left(2L-x + \frac{vt}{R}\right)^2\right]$$

$$+ \frac{v(y-v)}{(y+v)^2} \exp\left[\frac{(v+y)x - 2yL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) - yt}{2(DRt)^{1/2}}\right]$$

$$- \frac{v(y+v)}{(y-v)^2} \exp\left[\frac{(v-y)x + 2yL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) + yt}{2(DRt)^{1/2}}\right]$$

$$B_4(x) = 1 - \frac{(y-v)^2}{(y+v)^2} \exp(-yL/D)$$

B. Solutions for Zero-order Production Only

B1. Governing Equation (Steady-state)

$$D \frac{d^2 c}{dx^2} - v \frac{dc}{dx} + \gamma = 0$$

<u>Boundary Conditions</u>

$$c(0) = C_o$$

$$\frac{dc}{dx}(\infty) = \text{finite}$$

<u>Analytical Solution</u>

$$c(x) = C_o + \frac{\gamma x}{v}$$

B2. Governing Equation (Steady-state)

$$D \frac{d^2c}{dx^2} - v \frac{dc}{dx} + \gamma = 0$$

Boundary Conditions

$$\left(-D \frac{dc}{dx} + vc\right)\Bigg|_{x=0} = vC_o$$

$$\frac{dc}{dx}(\infty) = \text{finite}$$

Analytical Solution

$$c(x) = C_o + \frac{\gamma(vx+D)}{v^2}$$

B3. Governing Equation (Steady-state)

$$D \frac{d^2c}{dx^2} - v \frac{dc}{dx} + \gamma = 0$$

Boundary Conditions

$$c(0) = C_o$$

$$\frac{dc}{dx}(L) = 0$$

Analytical Solution

$$c(x) = C_o + \sum_{m=1}^{\infty} \frac{2\beta_m \sin(\frac{\beta_m x}{L}) \frac{\gamma L^2}{D} \exp(\frac{vx}{2D})}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{vL}{2D}] [\beta_m^2 + (\frac{vL}{2D})^2]}$$

where the eigenvalues β_m are the positive roots of

$$\beta_m \cot(\beta_m) + \frac{vL}{2D} = 0$$

The series solution converges too slowly to be of much use numerically. An alternative and more attractive solution is given by

$$c(x) = C_o + \frac{\gamma x}{v} + \frac{\gamma D}{v^2} \{\exp(- \frac{vL}{D}) - \exp[\frac{(x-L)v}{D}]\}$$

B4. Governing Equation (Steady-state)

$$D \frac{d^2c}{dx^2} - v \frac{dc}{dx} + \gamma = 0$$

Boundary Conditions

$$\left(-D \frac{dc}{dx} + vc\right)\Big|_{x=0} = vC_o$$

$$\frac{dc}{dx}(L) = 0$$

Analytical Solution

$$c(x) = C_o + \sum_{m=1}^{\infty} \frac{\left(\frac{2vL}{D}\right) \left(\frac{\gamma L^2}{D}\right) \beta_m \left[\beta_m \cos\left(\frac{\beta_m x}{L}\right) + \frac{vL}{2D} \sin\left(\frac{\beta_m x}{L}\right)\right] \exp\left(\frac{vx}{2D}\right)}{\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2 + \frac{vL}{D}\right] \left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2\right]^2}$$

where the eigenvalues β_m are the positive roots of

$$\beta_m \cot(\beta_m) - \frac{\beta_m^2 D}{vL} + \frac{vL}{4D} = 0$$

The series solution converges too slowly to be of much use numerically. An alternative and more attractive solution is given by

$$c(x) = C_o + \frac{\gamma x}{v} + \frac{\gamma D}{v^2} \left\{1 - \exp\left[\frac{v(x-L)}{D}\right]\right\}$$

B5. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} + \gamma$$

<u>Initial and Boundary Conditions</u>

$$c(x,0) = C_i$$

$$c(0,t) = \begin{cases} C_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(\infty,t) = \text{finite}$$

<u>Analytical Solution</u> (Carslaw and Jaeger *1959*, p. 388)

$$c(x,t) = \begin{cases} C_i + (C_o - C_i)\, A(x,t) + B(x,t) & 0 < t \leq t_o \\ C_i + (C_o - C_i)\, A(x,t) + B(x,t) - C_o\, A(x,t-t_o) & t > t_o \end{cases}$$

where

$$A(x,t) = \frac{1}{2}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \frac{1}{2}\exp(vx/D)\,\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$B(x,t) = \frac{\gamma}{R}\left\{t + \frac{(Rx-vt)}{2v}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] - \frac{(Rx + vt)}{2v}\exp(vx/D)\,\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]\right\}$$

B6. Governing Equation $R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} + \gamma$

Initial and Boundary Conditions

$$c(x,0) = C_i$$

$$\left(-D \frac{\partial c}{\partial x} + vc\right)\Big|_{x=0} = \begin{cases} vC_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(\infty,t) = \text{finite}$$

Analytical Solution (van Genuchten *1981*)

$$c(x,t) = \begin{cases} C_i + (C_o - C_i)\, A(x,t) + B(x,t) & 0 < t \leq t_o \\ C_i + (C_o - C_i)\, A(x,t) + B(x,t) - C_o\, A(x,t-t_o) & t > t_o \end{cases}$$

where

$$A(x,t) = \frac{1}{2}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \left(\frac{v^2 t}{\pi DR}\right)^{1/2} \exp\left[-\frac{(Rx - vt)^2}{4DRt}\right]$$
$$- \frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right) \exp(vx/D)\,\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$B(x,t) = \frac{\gamma}{R}\left\{t + \frac{1}{2v}\left(Rx - vt + \frac{DR}{v}\right)\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right]\right.$$
$$- \left(\frac{t}{4\pi DR}\right)^{1/2}\left(Rx + vt + \frac{2DR}{v}\right)\exp\left[-\frac{(Rx - vt)^2}{4DRt}\right]$$
$$\left. + \left[\frac{t}{2} - \frac{DR}{2v^2} + \frac{(Rx + vt)^2}{4DR}\right]\exp(vx/D)\,\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]\right\}$$

B7. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} + \gamma$$

Initial and Boundary Conditions

$$c(x,0) = C_i$$

$$c(0,t) = \begin{cases} C_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(L,t) = 0$$

Analytical Solution

$$c(x,t) = \begin{cases} C_i + (C_o - C_i)\, A(x,t) + B(x,t) & 0 < t \leq t_o \\ C_i + (C_o - C_i)\, A(x,t) + B(x,t) - C_o\, A(x,t-t_o) & t > t_o \end{cases}$$

where

$$A(x,t) = 1 - \sum_{m=1}^{\infty} E(\beta_m,x) \exp\left[\frac{vx}{2D} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}\right]$$

$$B(x,t) = B_1(x) - B_2(x,t)$$

$$B_1(x) = \sum_{m=1}^{\infty} \frac{E(\beta_m,x) \frac{\gamma L^2}{D} \exp\left(\frac{vx}{2D}\right)}{\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2\right]}$$

$$B_2(x,t) = \sum_{m=1}^{\infty} \frac{E(\beta_m,x) \frac{\gamma L^2}{D} \exp\left[\frac{vx}{2D} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}\right]}{\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2\right]}$$

and

$$E(\beta_m, x) = \frac{2\beta_m \sin(\frac{\beta_m x}{L})}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{vL}{2D}]}$$

The eigenvalues β_m are the positive roots of

$$\beta_m \cot(\beta_m) + \frac{vL}{2D} = 0$$

The term $B_1(x)$ in this solution converges much slower than the other terms. This term, however, can be expressed in an alternative form that is much easier to evaluate (see case B3):

$$B_1(x) = \frac{\gamma x}{v} + \frac{\gamma D}{v^2} \{\exp(-\frac{vL}{D}) - \exp[\frac{(x-L)v}{D}]\}$$

<u>Approximate Solution:</u>

$$A(x,t) = \frac{1}{2} \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \frac{1}{2} \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{1}{2} [2 + \frac{v(2L-x)}{D} + \frac{v^2 t}{DR}] \exp(vL/D) \operatorname{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$- (\frac{v^2 t}{\pi DR})^{1/2} \exp[\frac{vL}{D} - \frac{R}{4Dt} (2L-x + \frac{vt}{R})^2]$$

$$B(x,t) = \frac{\gamma}{R} \Bigg\{ t + \frac{(Rx-vt)}{2v} \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right]$$

$$- \frac{(Rx+vt)}{2v} \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$+ (\frac{t}{4\pi DR})^{1/2} [R(2L-x) + vt + \frac{2DR}{v}] \exp[\frac{vL}{D} - \frac{R}{4Dt}(2L-x + \frac{vt}{R})^2]$$

$$- [t + \frac{vR(2L-x)-DR}{2v^2} + \frac{R}{4D}(2L-x+\frac{vt}{R})^2] \exp(\frac{vL}{D}) \operatorname{erfc}\left[\frac{R(2L-x)+vt}{2(DRt)^{1/2}}\right]$$

$$- \frac{DR}{2v^2} \exp[\frac{v(x-L)}{D}] \operatorname{erfc}\left[\frac{R(2L-x)-vt}{2(DRt)^{1/2}}\right] \Bigg\}$$

B8. Governing Equations

$$R \frac{\partial C}{\partial T} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} + \gamma$$

<u>Initial and Boundary Conditions</u>

$$c(x,0) = C_i$$

$$\left(-D \frac{\partial c}{\partial x} + vc\right)\Big|_{x=0} = \begin{cases} VC_o & 0 < t \leqslant t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(L,t) = 0$$

<u>Analytical Solution</u>

$$c(x,t) = \begin{cases} C_i + (C_o - C_i)\, A(x,t) + B(x,t) & 0 < t \leqslant t_o \\ C_i + (C_o - C_i)\, A(x,t) + B(x,t) - C_o\, A(x,t-t_o) & t > t_o \end{cases}$$

where

$$A(x,t) = 1 - \sum_{m=1}^{\infty} E(\beta_m,x) \exp\left[\frac{vx}{2D} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}\right]$$

$$B(x,t) = B_1(x) - B_2(x,t)$$

$$B_1(x) = \sum_{m=1}^{\infty} \frac{E(\beta_m,x)\, \frac{\gamma L^2}{D} \exp\left(\frac{vx}{2D}\right)}{\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2\right]}$$

$$B_2(x) = \sum_{m=1}^{\infty} \frac{E(\beta_m,x)\, \frac{\gamma L^2}{D} \exp\left[\frac{vx}{2D} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}\right]}{\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2\right]}$$

and

$$E(\beta_m,x) = \frac{\frac{2vL}{D}\,\beta_m\,[\beta_m \cos(\frac{\beta_m x}{L}) + \frac{vL}{2D}\sin(\frac{\beta_m x}{L})]}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{vL}{D}]\,[\beta_m^2 + (\frac{vL}{2D})^2]}$$

The eigenvalues β_m are the positive roots of

$$\beta_m \cot(\beta_m) - \frac{\beta_m^2 D}{vL} + \frac{vL}{4D} = 0$$

The term $B_1(x)$, which also appears in the steady-state solution (case B4), converges much slower than the other terms in the series solution. This term, however, can be expressed in an alternative form that is much easier to evaluate:

$$B_1(x) = \frac{\gamma x}{v} + \frac{\gamma D}{v^2}\{1 - \exp[\frac{v(x-L)}{D}]\}$$

<u>Approximate Solution</u>

$$A(x,t) = \frac{1}{2}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + (\frac{v^2 t}{\pi DR})^{1/2} \exp[-\frac{(Rx - vt)^2}{4DRt}]$$

$$- \frac{1}{2}(1 + \frac{vx}{D} + \frac{v^2 t}{DR}) \exp(vx/D)\,\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$+ (\frac{4v^2 t}{\pi DR})^{1/2} [1 + \frac{v}{4D}(2L-x + \frac{vt}{R})] \exp[\frac{vL}{D} - \frac{R}{4Dt}(2L-x + \frac{vt}{R})^2]$$

$$- \frac{v}{D} [2L-x + \frac{3vt}{2R} + \frac{v}{4D}(2L-x + \frac{vt}{R})^2] \exp(vL/D)\,\mathrm{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$B(x,t) = \frac{\gamma}{R}\left\{ t + \frac{1}{2v}(Rx - vt + \frac{DR}{v})\ \mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] \right.$$

$$- (\frac{t}{4\pi DR})^{1/2}\ (Rx + vt + \frac{2DR}{v})\ \exp[- \frac{(Rx - vt)^2}{4DRt}]$$

$$+ [\frac{t}{2} - \frac{DR}{2v^2} + \frac{(Rx + vt)^2}{4DR}]\ \exp(vx/D)\ \mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$- \frac{DR}{2v^2}\ \exp[\frac{v(x-L)}{D}]\ \mathrm{erfc}\left[\frac{R(2L-x) - vt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{DR}{2v^2}\ [1 - \frac{v(2L-x)}{2D} + \frac{v^2}{2D^2}\ (2L-x + \frac{vt}{R})(2L-x + \frac{3vt}{R})$$

$$+ \frac{v^3}{6D^3}(2L-x + \frac{vt}{R})^3\ ]\ \exp(vL/D)\ \mathrm{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$- \frac{R}{v}\ [-1 + \frac{v}{2D}\ (2L-x + \frac{7vt}{3R}) + \frac{v^2}{6D^2}(2L-x + \frac{vt}{R})^2\ ]$$

$$\left. (\frac{Dt}{\pi R})^{1/2}\ \exp\ [\frac{vL}{D} - \frac{R}{4Dt}(2L-x + \frac{vt}{R})^2\ ] \right\}$$

B9. Governing Equation $R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} + \gamma$

Initial and Boundary Conditions

$$c(x,0) = C_i + \frac{\gamma x}{v}$$

$$c(0,t) = \begin{cases} C_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(\infty,t) = \text{finite}$$

Analytical Solution (Carslaw and Jaeger *1959*, p. 388)

$$c(x,t) = \begin{cases} C_i + \frac{\gamma x}{v} + (C_o - C_i)\, A(x,t) & 0 < t \leq t_o \\ C_i + \frac{\gamma x}{v} + (C_o - C_i)\, A(x,t) - C_o\, A(x,t-t_o) & t > t_o \end{cases}$$

where

$$A(x,t) = \frac{1}{2}\,\text{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \frac{1}{2}\exp(vx/D)\,\text{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

Comment: Note that the initial condition is of the same form as the steady-state solution for the same boundary conditions (case B1).

B10. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} + \gamma$$

Initial and Boundary Conditions

$$c(x,0) = C_i + \frac{\gamma(vx+D)}{v^2}$$

$$\left(-D \frac{\partial c}{\partial x} + vc\right)\Big|_{x=0} = \begin{cases} vC_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(\infty,t) = \text{finite}$$

Analytical Solution

$$c(x,t) = \begin{cases} C_i + \frac{\gamma(vx+D)}{v^2} + (C_o - C_i)\,A(x,t) & 0 < t \leq t_o \\ C_i + \frac{\gamma(vx+D)}{v^2} + (C_o - C_i)\,A(x,t) - C_o\,A(x,t-t_o) & t > t_o \end{cases}$$

where

$$A(x,t) = \frac{1}{2}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \left(\frac{v^2 t}{\pi DR}\right)^{1/2} \exp\left[-\frac{(Rx - vt)^2}{4DRt}\right]$$

$$- \frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right) \exp(vx/D)\,\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

Comment: Note that the initial condition is of the same form as the steady-state solution for the same boundary conditions (case B2).

B11. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} + \gamma$$

Initial Condition

$$c(x,0) \equiv A(x)$$

$$= C_i + \frac{\gamma x}{v} + \frac{\gamma D}{v^2} \{\exp(-\frac{vL}{D}) - \exp[\frac{v(x-L)}{D}]\}$$

Note that the initial condition is of the same form as the steady-state solution for the same boundary conditions (case B3).

Boundary Conditions

$$c(0,t) = \begin{cases} C_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(L,t) = 0$$

Analytical Solution

$$c(x,t) = \begin{cases} A(x) + (C_o - C_i)\, B(x,t) & 0 < t \leq t_o \\ A(x) + (C_o - C_i)\, B(x,t) - C_o\, B(x,t-t_o) & t > t_o \end{cases}$$

where A(x) is exactly the same as the initial condition, and where

$$B(x,t) = 1 - \sum_{m=1}^{\infty} \frac{2\, \beta_m \sin(\frac{\beta_m x}{L}) \exp[\frac{vx}{2D} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}]}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{vL}{2D}]}$$

The eigenvalues β_m are the positive roots of the equation

$$\beta_m \cot(\beta_m) + \frac{vL}{2D} = 0$$

Approximate Solution

$$A(x,t) = \frac{1}{2}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \frac{1}{2}\exp(vx/D)\,\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{1}{2}\left[2 + \frac{v(2L-x)}{D} + \frac{v^2 t}{DR}\right]\exp(vL/D)\,\mathrm{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$- \left(\frac{v^2 t}{\pi DR}\right)^{1/2}\exp\left[\frac{vL}{D} - \frac{R}{4Dt}\left(2L-x + \frac{vt}{R}\right)^2\right]$$

B12. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} + \gamma$$

Initial Condition

$$c(x,0) \equiv A(x)$$

$$= C_i + \frac{\gamma x}{v} + \frac{\gamma D}{v^2} \{1 - \exp[\frac{v(x-L)}{D}]\}$$

Note that the initial condition is of the same form as the steady-state solution for the same boundary conditions (case B4).

Boundary Conditions

$$(-D \frac{\partial c}{\partial x} + vc)\Big|_{x=0} = \begin{cases} C_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(L,t) = 0$$

Analytical Solution

$$c(x,t) = \begin{cases} A(x) + (C_o - C_i)\, B(x,t) & 0 < t \leq t_o \\ A(x) + (C_o - C_i)\, B(x,t) - C_o\, B(x,t-t_o) & t > t_o \end{cases}$$

where A(x) is exactly the same as the initial condition, and where

$$B(x,t) =$$

$$1 - \sum_{m=1}^{\infty} \frac{\frac{2vL}{D} \beta_m [\beta_m \cos(\frac{\beta_m x}{L}) + \frac{vL}{2D} \sin(\frac{\beta_m x}{L})] \exp[\frac{vx}{2D} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}]}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{vL}{D}]\, [\beta_m^2 + (\frac{vL}{2D})^2]}$$

The eigenvalues β_m are the positive roots of

$$\beta_m \cot(\beta_m) - \frac{\beta_m^2 D}{vL} + \frac{vL}{4D} = 0$$

Approximate Solution

$$B(x,t) = \frac{1}{2}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \left(\frac{v^2 t}{\pi DR}\right)^{1/2} \exp\left[-\frac{(Rx - vt)^2}{4DRt}\right]$$

$$- \frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right) \exp(vx/D)\,\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$+ \left(\frac{4v^2 t}{\pi DR}\right)^{1/2} \left[1 + \frac{v}{4D}\left(2L-x + \frac{vt}{R}\right)\right] \exp\left[\frac{vL}{D} - \frac{R}{4Dt}\left(2L-x + \frac{vt}{R}\right)^2\right]$$

$$- \frac{v}{D}\left[2L-x + \frac{3vt}{2R} + \frac{v}{4D}\left(2L-x + \frac{vt}{R}\right)^2\right] \exp(vL/D)\,\mathrm{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

B13. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} + \gamma$$

Initial and Boundary Conditions

$$c(x,0) = C_i$$

$$c(0,t) = C_a + C_b e^{-\lambda t}$$

$$\frac{\partial c}{\partial x}(\infty,t) = \text{finite}$$

Analytical Solution

$$c(x,t) = C_i + (C_a - C_i)\, A(x,t) + C_b\, B(x,t) + E(x,t)$$

where

$$A(x,t) = \frac{1}{2} \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \frac{1}{2} \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$B(x,t) = e^{-\lambda t} \left\{ \frac{1}{2} \exp\left[\frac{(v-y)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - yt}{2(DRt)^{1/2}}\right] + \frac{1}{2} \exp\left[\frac{(v+y)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + yt}{2(DRt)^{1/2}}\right] \right\}$$

$$E(x,t) = \frac{\gamma}{R} \left\{ t + \frac{(Rx-vt)}{2v} \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] - \frac{(Rx+vt)}{2v} \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right] \right\}$$

and

$$y = v\left(1 - \frac{4\lambda DR}{v^2}\right)^{1/2}$$

B14. Governing Equation $R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} + \gamma$

Initial and Boundary Conditions

$$c(x,0) = C_i$$

$$\left(-D \frac{\partial c}{\partial x} + vc\right)\Big|_{x=0} = v(C_a + C_b e^{-\lambda t})$$

$$\frac{\partial c}{\partial x}(\infty,t) = \text{finite}$$

Analytical Solution

$$c(x,t) = C_i + (C_a - C_i) A(x,t) + C_b B(x,t) + E(x,t)$$

where

$$A(x,t) = \frac{1}{2} \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \left(\frac{v^2 t}{\pi DR}\right)^{1/2} \exp\left[-\frac{(Rx - vt)^2}{4DRt}\right]$$

$$- \frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right) \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$B(x,t) = e^{-\lambda t}\left\{\frac{v}{(v+y)} \exp\left[\frac{(v-y)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - yt}{2(DRt)^{1/2}}\right]\right.$$

$$\left. + \frac{v}{(v-y)} \exp\left[\frac{(v+y)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + yt}{2(DRt)^{1/2}}\right]\right\}$$

$$- \frac{v^2}{2\lambda DR} \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$E(x,t) = \frac{\gamma}{R}\left\{ t + \frac{1}{2v}(Rx - vt + \frac{DR}{v}) \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right]\right.$$

$$- (\frac{t}{4\pi DR})^{1/2} (Rx + vt + \frac{2DR}{v}) \exp[- \frac{(Rx - vt)^2}{4DRt}]$$

$$\left. + [\frac{t}{2} - \frac{DR}{2v^2} + \frac{(Rx + vt)^2}{4DR}] \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]\right\}$$

and

$$y = v\ (1 - \frac{4\lambda DR}{v^2})^{1/2}$$

B15. Governing Equation $$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} + \gamma$$

Initial and Boundary Conditions

$$c(x,0) = C_i$$

$$c(0,t) = C_a + C_b e^{-\lambda t}$$

$$\frac{\partial c}{\partial x}(L,t) = 0$$

Analytical Solution

$$c(x,t) = C_i + (C_a - C_i) A(x,t) + C_b B(x,t) + F(x,t)$$

where

$$A(x,t) = 1 - \sum_{m=1}^{\infty} E(\beta_m,x) \exp[\frac{vx}{2D} - \frac{v^2 t}{4DR} - \frac{\beta_m Dt}{L^2 R}]$$

$$B(x,t) = e^{-\lambda t} [B_1(x) - B_2(x,t)]$$

$$B_1(x) = 1 + \sum_{m=1}^{\infty} \frac{E(\beta_m,x) \frac{\lambda L^2 R}{D} \exp(\frac{vx}{2D})}{[\beta_m^2 + (\frac{vL}{2D})^2 - \frac{\lambda L^2 R}{D}]}$$

$$B_2(x,t) = \sum_{m=1}^{\infty} \frac{E(\beta_m,x) [\beta_m^2 + (\frac{vL}{2D})^2] \exp[\frac{vx}{2D} + \lambda t - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}]}{[\beta_m^2 + (\frac{vL}{2D})^2 - \frac{\lambda L^2 R}{D}]}$$

$$F(x,t) = F_1(x) - F_2(x,t)$$

$$F_1(x) = \sum_{m=1}^{\infty} \frac{E(\beta_m, x)\, \frac{\gamma L^2}{D} \exp(\frac{vx}{2D})}{[\beta_m^2 + (\frac{vL}{2D})^2]}$$

$$F_2(x,t) = \sum_{m=1}^{\infty} \frac{E(\beta_m, x)\, \frac{\gamma L^2}{D} \exp[\frac{vx}{2D} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}]}{[\beta_m^2 + (\frac{vL}{2D})^2]}$$

and

$$E(\beta_m, x) = \frac{2\beta_m \sin(\frac{\beta_m x}{L})}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{vL}{2D}]}$$

The eigenvalues β_m are the positive roots of

$$\beta_m \cot(\beta_m) + \frac{vL}{2D} = 0$$

The terms $B_1(x)$ and $F_1(x)$ converge much slower than the other terms in the series solution. Both terms, however, can be expressed in alternative forms that are much easier to evaluate:

$$B_1(x) = \frac{\exp[\frac{(v-y)x}{2D}] + (\frac{y-v}{y+v}) \exp[\frac{(v+y)x-2yL}{2D}]}{[1 + (\frac{y-v}{y+v}) \exp(-yL/D)]}$$

where

$$y = v\ (1 - \frac{4\lambda DR}{v^2})^{1/2}$$

and

$$F_1(x) = \frac{\gamma x}{v} + \frac{\gamma D}{v^2} \{\exp(-\frac{vL}{D}) - \exp[\frac{v(x-L)}{D}]\}$$

Approximate Solution

$$A(x,t) = \frac{1}{2}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \frac{1}{2}\exp(vx/D)\,\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{1}{2}\left[2 + \frac{v(2L-x)}{D} + \frac{v^2 t}{DR}\right]\exp(vL/D)\,\mathrm{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$- \left(\frac{v^2 t}{\pi DR}\right)^{1/2} \exp\left[\frac{vL}{D} - \frac{R}{4Dt}\left(2L-x + \frac{vt}{R}\right)^2\right]$$

$$B(x,t) = e^{-\lambda t}\, B_3(x,t)/B_4(x)$$

$$B_3(x,t) = \frac{1}{2}\exp\left[\frac{(v-y)x}{2D}\right]\mathrm{erfc}\left[\frac{Rx - yt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{1}{2}\exp\left[\frac{(v+y)x}{2D}\right]\mathrm{erfc}\left[\frac{Rx + yt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{(y-v)}{2(y+v)}\exp\left[\frac{(v+y)x-2yL}{2D}\right]\mathrm{erfc}\left[\frac{R(2L-x) - yt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{(y+v)}{2(y-v)}\exp\left[\frac{(v-y)x+2yL}{2D}\right]\mathrm{erfc}\left[\frac{R(2L-x) + yt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v^2}{2\lambda DR}\exp\left(\frac{vL}{D} + \lambda t\right)\mathrm{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$B_4(x) = 1 + \left(\frac{y-v}{y+v}\right)\exp(-yL/D)$$

and

$$F(x,t) = \frac{\gamma}{R}\left\{t + \frac{(Rx-vt)}{2v}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right]\right.$$

$$\left. - \frac{(Rx+vt)}{2v}\exp(vx/D)\,\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]\right.$$

$$+ \left(\frac{t}{4\pi DR}\right)^{1/2} \left[R(2L-x) + vt + \frac{2DR}{v}\right] \exp\left[\frac{vL}{D} - \frac{R}{4Dt}\left(2L-x + \frac{vt}{R}\right)^2\right]$$

$$- \left[t + \frac{vR(2L-x)-DR}{2v^2} + \frac{R}{4D}\left(2L-x + \frac{vt}{R}\right)^2\right] \exp\left(\frac{vL}{D}\right) \operatorname{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$- \frac{DR}{2v^2} \exp\left[\frac{v(x-L)}{D}\right] \operatorname{erfc}\left[\frac{R(2L-x) - vt}{2(DRt)^{1/2}}\right]\Bigg\}$$

B16. Governing Equation $R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} + \gamma$

Initial and Boundary Conditions

$$c(x,0) = C_i$$

$$\left(-D \frac{\partial c}{\partial x} + vc\right)\Big|_{x=0} = v(C_a + C_b\, e^{-\lambda t})$$

$$\frac{\partial c}{\partial x}(L,t) = 0$$

Analytical Solution

$$c(x,t) = C_i + (C_a - C_i)\, A(x,t) + C_b\, B(x,t) + F(x,t)$$

where

$$A(x,t) = 1 - \sum_{m=1}^{\infty} E(\beta_m,x) \exp\left[\frac{vx}{2D} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}\right]$$

$$B(x,t) = e^{-\lambda t}\, [B_1(x) - B_2(x,t)]$$

$$B_1(x) = 1 + \sum_{m=1}^{\infty} \frac{E(\beta_m,x)\, \frac{\lambda L^2}{D} \exp\left(\frac{vx}{2D}\right)}{\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2 - \frac{\lambda L^2 R}{D}\right]}$$

$$B_2(x,t) = \sum_{m=1}^{\infty} \frac{E(\beta_m,x)\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2\right] \exp\left[\frac{vx}{2D} + \lambda t - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}\right]}{\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2 - \frac{\lambda L^2 R}{D}\right]}$$

$$F(x,t) = F_1(x) - F_2(x,t)$$

$$F_1(x) = \sum_{m=1}^{\infty} \frac{E(\beta_m,x)\ \frac{\gamma L^2}{D}\ \exp(\frac{vx}{2D})}{[\beta_m^2 + (\frac{vL}{2D})^2]}$$

$$F_2(x,t) = \sum_{m=1}^{\infty} \frac{E(\beta_m,x)\ \frac{\gamma L^2}{D}\ \exp[\frac{vx}{2D} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}]}{[\beta_m^2 + (\frac{vL}{2D})^2]}$$

and

$$E(\beta_m,x) = \frac{\frac{2vL}{D}\ \beta_m\ [\beta_m \cos(\frac{\beta_m x}{L}) + \frac{vL}{2D} \sin(\frac{\beta_m x}{L})]}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{vL}{D}]\ [\beta_m^2 + (\frac{vL}{2D})^2]}$$

The eigenvalues β_m are the positive roots of

$$\beta_m \cot(\beta_m) - \frac{\beta_m^2 D}{vL} + \frac{vL}{4D} = 0$$

The terms $B_1(x)$ and $F_1(x)$ converge much slower than the other terms in the series solution. Both $B_1(x)$ and $F_1(x)$, however, can be expressed in alternative forms that are much easier to evaluate:

$$B_1(x) = \frac{\exp[\frac{(v-y)x}{2D}] + (\frac{y-v}{y+v})\ \exp[\frac{(v+y)x-2yL}{2D}]}{[\frac{y+v}{2v} - \frac{(y-v)^2}{2v(y+v)}\ \exp(-yL/D)]}$$

where

$$y = v\ (1 - \frac{4\lambda DR}{v^2})^{1/2}$$

and

$$F_1(x) = \frac{\gamma x}{v} + \frac{\gamma D}{v^2}\ \{1 - \exp[\frac{v(x-L)}{D}]\}$$

Approximate Solution

$$A(x,t) = \frac{1}{2}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \left(\frac{v^2 t}{\pi DR}\right)^{1/2} \exp\left[-\frac{(Rx - vt)^2}{4DRt}\right]$$

$$- \frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right) \exp(vx/D)\,\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$+ \left(\frac{4v^2 t}{\pi DR}\right)^{1/2} \left[1 + \frac{v}{4D}\left(2L-x + \frac{vt}{R}\right)\right] \exp\left[\frac{vL}{D} - \frac{R}{4Dt}\left(2L-x + \frac{vt}{R}\right)^2\right]$$

$$- \frac{v}{D}\left[2L-x + \frac{3vt}{2R} + \frac{v}{4D}\left(2L-x + \frac{vt}{R}\right)^2\right] \exp(vL/D)\,\mathrm{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$B(x,t) = e^{-\lambda t}\, B_3(x,t)/B_4(x)$$

$$B_3(x,t) = \left(\frac{v}{v+y}\right) \exp\left[\frac{(v-y)x}{2D}\right] \mathrm{erfc}\left[\frac{Rx - yt}{2(DRt)^{1/2}}\right]$$

$$+ \left(\frac{v}{v-y}\right) \exp\left[\frac{(v+y)x}{2D}\right] \mathrm{erfc}\left[\frac{Rx + yt}{2(DRt)^{1/2}}\right]$$

$$- \frac{v^2}{2\lambda DR} \exp\left(\frac{vx}{D} + \lambda t\right) \mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$- \frac{v^2}{2\lambda DR}\left[\frac{v(2L-x)}{D} + \frac{v^2 t}{DR} + 3 - \frac{v^2}{\lambda DR}\right] \exp\left(\frac{vL}{D} + \lambda t\right) \mathrm{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v^3}{\lambda DR}\left(\frac{t}{\pi DR}\right)^{1/2} \exp\left[\frac{vL}{D} + \lambda t - \frac{R}{4Dt}\left(2L-x + \frac{vt}{R}\right)^2\right]$$

$$+ \frac{v(y-v)}{(y+v)^2} \exp\left[\frac{(v+y)x-2yL}{2D}\right] \mathrm{erfc}\left[\frac{R(2L-x) - yt}{2(DRt)^{1/2}}\right]$$

$$- \frac{v(y+v)}{(y-v)^2} \exp\left[\frac{(v-y)x+2yL}{2D}\right] \mathrm{erfc}\left[\frac{R(2L-x) + yt}{2(DRt)^{1/2}}\right]$$

$$B_4(x) = 1 - \frac{(y-v)^2}{(y+v)^2} \exp(-yL/D)$$

and

$$F(x,t) = \frac{\gamma}{R} \left\{ t + \frac{1}{2v}(Rx - vt + \frac{DR}{v}) \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] \right.$$

$$- (\frac{t}{4\pi DR})^{1/2} (Rx + vt + \frac{2DR}{v}) \exp[- \frac{(Rx - vt)^2}{4DRt}]$$

$$+ [\frac{t}{2} - \frac{DR}{2v^2} + \frac{(Rx + vt)^2}{4DR}] \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$- \frac{DR}{2v^2} \exp[\frac{v(x-L)}{D}] \operatorname{erfc}\left[\frac{R(2L-x) - vt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{DR}{2v^2} [1 - \frac{v(2L-x)}{2D} + \frac{v^2}{2D^2}(2L-x + \frac{vt}{R})(2L-x + \frac{3vt}{R})$$

$$+ \frac{v^3}{6D^3}(2L-x + \frac{vt}{R})^3] \exp(vL/D) \operatorname{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$- \frac{R}{v} [-1 + \frac{v}{2D}(2L-x + \frac{7vt}{3R}) + \frac{v^2}{6D^2}(2L-x + \frac{vt}{R})^2]$$

$$\left. (\frac{Dt}{\pi R})^{1/2} \exp[\frac{vL}{D} - \frac{R}{4Dt}(2L-x + \frac{vt}{R})^2] \right\}$$

C. Solutions for Simultaneous Zero-order Production and First-order Decay

C1. Governing Equation (Steady-state)

$$D \frac{d^2c}{dx^2} - v \frac{dc}{dx} - \mu c + \gamma = 0$$

Boundary Conditions

$$c(0) = C_o$$

$$\frac{dc}{dx}(\infty) = 0$$

Analytical Solution

$$c(x) = \frac{\gamma}{\mu} + (C_o - \frac{\gamma}{\mu}) \exp[\frac{(v-u)x}{2D}]$$

where

$$u = v \, (1 + \frac{4\mu D}{v^2})^{1/2}$$

C2. Governing Equation (Steady-state)

$$D \frac{d^2c}{dx^2} - v \frac{dc}{dx} - \mu c + \gamma = 0$$

Boundary Conditions

$$\left(-D \frac{dc}{dx} + vc\right)\Big|_{x=0} = vC_o$$

$$\frac{dc}{dx}(\infty) = 0$$

Analytical Solution (Gershon and Nir *1969*)

$$c(x) = \frac{\gamma}{\mu} + \left(C_o - \frac{\gamma}{\mu}\right) \frac{2v}{u+v} \exp\left[\frac{(v-u)x}{2D}\right]$$

where

$$u = v \left(1 + \frac{4\mu D}{v^2}\right)^{1/2}$$

C3. Governing Equation (Steady-state)

$$D \frac{d^2c}{dx^2} - v \frac{dc}{dx} - \mu c + \gamma = 0$$

Boundary Conditions

$$c(0) = C_o$$

$$\frac{dc}{dx}(L) = 0$$

Analytical Solution

$$c(x) = \frac{\gamma}{\mu} + (C_o - \frac{\gamma}{\mu})\, A(x)$$

where

$$A(x) = 1 - \sum_{m=1}^{\infty} \frac{2\beta_m \sin(\frac{\beta_m x}{L}) \frac{\mu L^2}{D} \exp(\frac{vx}{2D})}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{vL}{2D}]\ [\beta_m^2 + (\frac{vL}{2D})^2 + \frac{\mu L^2}{D}]}$$

and where the eigenvalues β_m are the positive roots of

$$\beta_m \cot(\beta_m) + \frac{vL}{2D} = 0.$$

The above series solution converges too slowly to be of much use numerically. The following equivalent expression for A(x) is much easier to evaluate

$$A(x) = \frac{\exp[\frac{(v-u)x}{2D}] + (\frac{u-v}{u+v}) \exp[\frac{(v+u)x}{2D} - \frac{uL}{D}]}{[1 + (\frac{u-v}{u+v}) \exp(-uL/D)]}$$

where

$$u = v\ (1 + \frac{4\mu D}{v^2})^{1/2}$$

C4. Governing Equation (Steady-state)

$$D \frac{d^2c}{dx^2} - v \frac{dc}{dx} - \mu c + \gamma = 0$$

<u>Boundary Conditions</u>

$$\left(-D \frac{dc}{dx} + vc\right)\Big|_{x=0} = vC_o$$

$$\frac{dc}{dx}(L) = 0$$

<u>Analytical Solution</u>

$$c(x) = \frac{\gamma}{\mu} + \left(C_o - \frac{\gamma}{\mu}\right) A(x)$$

where

$$A(x) =$$

$$1 - \sum_{m=1}^{\infty} \frac{\left(\frac{2vL}{D}\right)\left(\frac{\mu L^2}{D}\right) \beta_m \left[\beta_m \cos\left(\frac{\beta_m x}{L}\right) + \frac{vL}{2D} \sin\left(\frac{\beta_m x}{L}\right)\right] \exp\left(\frac{vx}{2D}\right)}{\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2 + \frac{vL}{D}\right]\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2\right]\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2 + \frac{\mu L^2}{D}\right]}$$

and where the eigenvalues β_m are the positive roots of

$$\beta_m \cot(\beta_m) - \frac{\beta_m^2 D}{vL} + \frac{vL}{4D} = 0$$

The above series solution converges too slowly to be of much use numerically. The following equivalent expression for A(x) is much easier to use (see also Gershon and Nir *1969*)

$$A(x) = \frac{\exp\left[\frac{(v-u)x}{2D}\right] + \left(\frac{u-v}{u+v}\right) \exp\left[\frac{(v+u)x - 2uL}{2D}\right]}{\left[\frac{u+v}{2v} - \frac{(u-v)^2}{2v(u+v)} \exp(-uL/D)\right]}$$

where

$$u = v\left(1 + \frac{4\mu D}{v^2}\right)^{1/2}$$

C5. Governing Equation $$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} - \mu c + \gamma$$

<u>Initial and Boundary Conditions</u>

$$c(x,0) = C_i$$

$$c(0,t) = \begin{cases} C_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(\infty,t) = 0$$

<u>Analytical Solution</u> (van Genuchten *1981*; see also Bear *1972*, p. 630)

$$c(x,t) =$$

$$\begin{cases} \frac{\gamma}{\mu} + (C_i - \frac{\gamma}{\mu})\, A(x,t) + (C_o - \frac{\gamma}{\mu})\, B(x,t) & 0 < t \leq t_o \\ \frac{\gamma}{\mu} + (C_i - \frac{\gamma}{\mu})\, A(x,t) + (C_o - \frac{\gamma}{\mu})\, B(x,t) - C_o\, B(x,t-t_o) & t > t_o \end{cases}$$

where

$$A(x,t) = \exp(-\mu t/R) \left\{ 1 - \frac{1}{2} \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] - \frac{1}{2} \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right] \right\}$$

$$B(x,t) = \frac{1}{2} \exp\left[\frac{(v-u)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - ut}{2(DRt)^{1/2}}\right] + \frac{1}{2} \exp\left[\frac{(v+u)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + ut}{2(DRt)^{1/2}}\right]$$

and $$u = v \left(1 + \frac{4\mu D}{v^2}\right)^{1/2}$$

C6. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} - \mu c + \gamma$$

Initial and Boundary Conditions

$$c(x,0) = C_i$$

$$\left(-D \frac{\partial c}{\partial x} + vc\right)\Big|_{x=0} = \begin{cases} vC_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(\infty,t) = 0$$

Analytical Solution (van Genuchten *1981*; see also Parlange and Starr *1978*)

$$c(x,t) =$$

$$\begin{cases} \frac{\gamma}{\mu} + (C_i - \frac{\gamma}{\mu})\, A(x,t) + (C_o - \frac{\gamma}{\mu})\, B(x,t) & 0 < t \leq t_o \\ \frac{\gamma}{\mu} + (C_i - \frac{\gamma}{\mu})\, A(x,t) + (C_o - \frac{\gamma}{\mu})\, B(x,t) - C_o\, B(x,t-t_o) & t > t_o \end{cases}$$

where

$$A(x,t) = \exp(-\mu t/R) \left\{ 1 - \frac{1}{2}\, \mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] - \left(\frac{v^2 t}{\pi DR}\right)^{1/2} \exp\left[-\frac{(Rx - vt)^2}{4DRt}\right] + \frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right) \exp(vx/D)\, \mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right] \right\}$$

$$B(x,t) = \frac{v}{(v+u)} \exp\left[\frac{(v-u)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v}{(v-u)} \exp\left[\frac{(v+u)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v^2}{2\mu D} \exp\left(\frac{vx}{D} - \frac{\mu t}{R}\right) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

and

$$u = v \left(1 + \frac{4\mu D}{v^2}\right)^{1/2}$$

C7. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} - \mu c + \gamma$$

<u>Initial and Boundary Conditions</u>

$$c(x,0) = C_i$$

$$c(0,t) = \begin{cases} C_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(L,t) = 0$$

<u>Analytical Solution</u> (Selim and Mansell *1976*)

$$c(x,t) =$$

$$\begin{cases} \frac{\gamma}{\mu} + (C_i - \frac{\gamma}{\mu}) A(x,t) + (C_o - \frac{\gamma}{\mu}) B(x,t) & 0 < t \leq t_o \\ \frac{\gamma}{\mu} + (C_i - \frac{\gamma}{\mu}) A(x,t) + (C_o - \frac{\gamma}{\mu}) B(x,t) - C_o B(x,t-t_o) & t > t_o \end{cases}$$

where

$$A(x,t) = \sum_{m=1}^{\infty} E(\beta_m,x) \exp\left[\frac{vx}{2D} - \frac{\mu t}{R} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}\right]$$

$$B(x,t) = B_1(x) - B_2(x,t)$$

$$B_1(x) = 1 - \sum_{m=1}^{\infty} \frac{E(\beta_m,x) \frac{\mu L^2}{D} \exp(\frac{vx}{2D})}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{\mu L^2}{D}]}$$

$$B_2(x,t) = \sum_{m=1}^{\infty} \frac{E(\beta_m,x) [\beta_m^2 + (\frac{vL}{2D})^2] \exp[\frac{vx}{2D} - \frac{\mu t}{R} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}]}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{\mu L^2}{D}]}$$

and

$$E(\beta_m,x) = \frac{2\beta_m \sin(\frac{\beta_m x}{L})}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{vL}{2D}]}$$

The eigenvalues β_m are the positive roots of

$$\beta_m \cot(\beta_m) + \frac{vL}{2D} = 0$$

The term $B_1(x)$, which also appears in the steady-state solution (case C3), converges much slower than the other terms in the solution. This term, however, can be expressed in an alternative form that is much easier to evaluate:

$$B_1(x) = \frac{\exp[\frac{(v-u)x}{2D}] + (\frac{u-v}{u+v}) \exp[\frac{(v+u)x}{2D} - \frac{uL}{D}]}{[1 + (\frac{u-v}{u+v}) \exp(-uL/D)]}$$

Approximate Solution

$$A(x,t) = \exp(-\mu t/R) \Bigg\{ 1 - \frac{1}{2} \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right]$$

$$- \frac{1}{2} \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$- \frac{1}{2} [2 + \frac{v(2L-x)}{D} + \frac{v^2 t}{DR}] \exp(vL/D) \operatorname{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$+ (\frac{v^2 t}{\pi DR})^{1/2} \exp[\frac{vL}{D} - \frac{R}{4Dt}(2L-x + \frac{vt}{R})^2] \Bigg\}$$

$$B(x,t) = B_3(x,t)/B_4(x)$$

where

$$B_3(x,t) = \frac{1}{2}\exp\left[\frac{(v-u)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{1}{2}\exp\left[\frac{(v+u)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{(u-v)}{2(u+v)}\exp\left[\frac{(v+u)x - 2uL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) - ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{(u+v)}{2(u-v)}\exp\left[\frac{(v-u)x + 2uL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) + ut}{2(DRt)^{1/2}}\right]$$

$$- \frac{v^2}{2\mu D}\exp\left(\frac{vL}{D} - \frac{\mu t}{R}\right) \operatorname{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$B_4(x) = 1 + \left(\frac{u-v}{u+v}\right)\exp(-uL/D)$$

and

$$u = v\left(1 + \frac{4\mu D}{v^2}\right)^{1/2}$$

C8. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} - \mu c + \gamma$$

Initial and Boundary Conditions

$$c(x,0) = C_i$$

$$\left(-D \frac{\partial c}{\partial x} + vc\right)\Bigg|_{x=0} = \begin{cases} vC_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(L,t) = 0$$

Analytical Solution

$$c(x,t) =$$

$$\begin{cases} \frac{\gamma}{\mu} + (C_i - \frac{\gamma}{\mu})\, A(x,t) + (C_o - \frac{\gamma}{\mu})\, B(x,t) & 0 < t \leq t_o \\ \frac{\gamma}{\mu} + (C_i - \frac{\gamma}{\mu})\, A(x,t) + (C_o - \frac{\gamma}{\mu})\, B(x,t) - C_o\, B(x,t-t_o) & t > t_o \end{cases}$$

where

$$A(x,t) = \sum_{m=1}^{\infty} E(\beta_m,x) \exp\left[\frac{vx}{2D} - \frac{\mu t}{R} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 D t}{L^2 R}\right]$$

$$B(x,t) = B_1(x) - B_2(x,t)$$

$$B_1(x) = 1 - \frac{\mu L^2}{D} \sum_{m=1}^{\infty} \frac{E(\beta_m,x) \exp(\frac{vx}{2D})}{\left[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{\mu L^2}{D}\right]}$$

$$B_2(x,t) = \sum_{m=1}^{\infty} \frac{E(\beta_m,x) \left[\beta_m^2 + (\frac{vL}{2D})^2\right] \exp\left[\frac{vx}{2D} - \frac{\mu t}{R} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 D t}{L^2 R}\right]}{\left[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{\mu L^2}{D}\right]}$$

and

$$E(\beta_m,x) = \frac{\frac{2vL}{D}\,\beta_m\left[\cos\left(\frac{\beta_m x}{L}\right) + \frac{vL}{2D}\sin\left(\frac{\beta_m x}{L}\right)\right]}{\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2 + \frac{vL}{D}\right]\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2\right]}$$

The eigenvalues β_m are the positive roots of

$$\beta_m \cot(\beta_m) - \frac{\beta_m^2 D}{vL} + \frac{vL}{4D} = 0$$

The term $B_1(x)$, which also appears in the steady-state solution (case C4), converges much slower than the other terms in the series solution. This term, however, can be expressed in an alternative form that is much easier to evaluate:

$$B_1(x) = \frac{\exp\left[\frac{(v-u)x}{2D}\right] + \left(\frac{u-v}{u+v}\right)\exp\left[\frac{(v+u)x - 2uL}{2D}\right]}{\left[\frac{u+v}{2v} - \frac{(u-v)^2}{2v(u+v)}\exp(-uL/D)\right]}$$

<u>Approximate Solution</u>

$$\begin{aligned}
A(x,t) = \exp(-\mu t/R)\Bigg\{1 &- \frac{1}{2}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] - \left(\frac{v^2 t}{\pi DR}\right)^{1/2}\exp\left[-\frac{(Rx - vt)^2}{4DRt}\right] \\
&+ \frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right)\exp(vx/D)\,\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right] \\
&- \left(\frac{4v^2 t}{\pi DR}\right)^{1/2}\left[1 + \frac{v}{4D}\left(2L-x + \frac{vt}{R}\right)\right]\exp\left[\frac{vL}{D} - \frac{R}{4Dt}\left(2L-x + \frac{vt}{R}\right)^2\right] \\
&+ \frac{v}{D}\left[2L-x + \frac{3vt}{2R} + \frac{v}{4D}\left(2L-x + \frac{vt}{R}\right)^2\right]\exp(vL/D)\,\mathrm{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]\Bigg\}
\end{aligned}$$

$$B(x,t) = B_3(x,t)/B_4(x,t)$$

where

$$B_3(x,t) = \frac{v}{(v+u)} \exp[\frac{(v-u)x}{2D}] \operatorname{erfc}\left[\frac{Rx - ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v}{(v-u)} \exp[\frac{(v+u)x}{2D}] \operatorname{erfc}\left[\frac{Rx + ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v^2}{2\mu D} \exp(\frac{vx}{D} - \frac{\mu t}{R}) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v^2}{2\mu D} [\frac{v(2L-x)}{D} + \frac{v^2 t}{DR} + 3 + \frac{v^2}{\mu D}] \exp(\frac{vL}{D} - \frac{\mu t}{R}) \operatorname{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$- \frac{v^3}{\mu D} (\frac{t}{\pi DR})^{1/2} \exp[\frac{vL}{D} - \frac{\mu t}{R} - \frac{R}{4Dt}(2L-x + \frac{vt}{R})^2]$$

$$+ \frac{v(u-v)}{(u+v)^2} \exp[\frac{(v+u)x - 2uL}{2D}] \operatorname{erfc}\left[\frac{R(2L-x) - ut}{2(DRt)^{1/2}}\right]$$

$$- \frac{v(u+v)}{(u-v)^2} \exp[\frac{(v-u)x + 2uL}{2D}] \operatorname{erfc}\left[\frac{R(2L-x) + ut}{2(DRt)^{1/2}}\right]$$

$$B_4(x) = 1 - \frac{(u-v)^2}{(u+v)^2} \exp(-uL/D)$$

and

$$u = v\ (1 + \frac{4\mu D}{v^2})^{1/2}$$

C9. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} - \mu c + \gamma$$

Initial Condition

$$c(x,0) \equiv A(x)$$

$$= \frac{\gamma}{\mu} + (C_i - \frac{\gamma}{\mu}) \exp \left[\frac{(v-u)x}{2D}\right]$$

where

$$u = v \left(1 + \frac{4\mu D}{v^2}\right)^{1/2}$$

Note that the initial condition is of the same form as the steady-state solution for the same boundary conditions (case C1).

Boundary Conditions

$$c(0,t) = \begin{cases} C_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(\infty,t) = 0$$

Analytical Solution

$$c(x,t) = \begin{cases} A(x) + (C_o - C_i)\, B(x,t) & 0 < t \leq t_o \\ A(x) + (C_o - C_i)\, B(x,t) - C_o\, B(x,t-t_o) & t > t_o \end{cases}$$

where A(x) is the same as the initial condition, and where

$$B(x,t) = \frac{1}{2} \exp\left[\frac{(v-u)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{1}{2} \exp\left[\frac{(v+u)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + ut}{2(DRt)^{1/2}}\right]$$

C10. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} - \mu c + \gamma$$

Initial Condition

$$c(x,0) \equiv A(x)$$

$$= \frac{\gamma}{\mu} + (C_i - \frac{\gamma}{\mu}) \frac{2v}{v+u} \exp[\frac{(v-u)x}{2D}]$$

where

$$u = v\, (1 + \frac{4\mu D}{v^2})^{1/2}$$

Note that the initial condition is of the same form as the steady-state solution for the same boundary conditions (case C2).

Boundary Conditions

$$(-D \frac{\partial c}{\partial x} + vc)\Big|_{x=0} = \begin{cases} vC_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x} (\infty,t) = 0$$

Analytical Solution

$$c(x,t) = \begin{cases} A(x) + (C_o - C_i)\, B(x,t) & 0 < t \leq t_o \\ A(x) + (C_o - C_i)\, B(x,t) - C_o\, B(x,t-t_o) & t > t_o \end{cases}$$

where A(x) is the same as the initial condition, and where

$$B(x,t) = \frac{v}{(v+u)} \exp[\frac{(v-u)x}{2D}]\ \mathrm{erfc}\left[\frac{Rx - ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v}{(v-u)} \exp[\frac{(v+u)x}{2D}]\ \mathrm{erfc}\left[\frac{Rx + ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v^2}{2\mu D} \exp(\frac{vx}{D} - \frac{\mu t}{R})\ \mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

C11. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} - \mu c + \gamma$$

Initial Condition

$$c(x,0) \equiv A(x)$$

$$= \frac{\gamma}{\mu} + (C_i - \frac{\gamma}{\mu}) \frac{\exp[\frac{(v-u)x}{2D}] + (\frac{u-v}{u+v}) \exp[\frac{(v+u)x - 2uL}{2D}]}{[1 + (\frac{u-v}{u+v}) \exp(-uL/D)]}$$

where

$$u = v \left(1 + \frac{4\mu D}{v^2}\right)^{1/2}$$

Note that the initial condition is of the same form as the steady-state solution for the same boundary conditions (case C3).

Boundary Conditions

$$c(0,t) = \begin{cases} C_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(L,t) = 0$$

Analytical Solution

$$c(x,t) = \begin{cases} A(x) + (C_o - C_i)\, B(x,t) & 0 < t \leq t_o \\ A(x) + (C_o - C_i)\, B(x,t) - C_o\, B(x,t-t_o) & t > t_o \end{cases}$$

where A(x) is exactly the initial condition, and where

$$B(x,t) = B_1(x) - B_2(x,t)$$

with

$$B_1(x) = 1 - \sum_{m=1}^{\infty} \frac{E(\beta_m,x)\,\frac{\mu L^2}{D}\,\exp(\frac{vx}{2D})}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{\mu L^2}{D}]}$$

$$B_2(x,t) = \sum_{m=1}^{\infty} \frac{E(\beta_m,x)\,[\beta_m^2 + (\frac{vL}{2D})^2]\,\exp[\frac{vx}{2D} - \frac{\mu t}{R} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}]}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{\mu L^2}{D}]}$$

and

$$E(\beta_m,x) = \frac{2\beta_m \sin(\frac{\beta_m x}{L})}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{vL}{2D}]}$$

The eigenvalues β_m are the positive roots of

$$\beta_m \cot(\beta_m) + \frac{vL}{2D} = 0$$

The term $B_1(x)$, which also appears in the steady-state solution (case C3), converges much slower than the other terms in the solution. This term, however, can be expressed in an alternative form that is much easier to evaluate:

$$B_1(x) = \frac{\exp[\frac{(v-u)x}{2D}] + (\frac{u-v}{u+v})\exp[\frac{(v+u)x}{2D} - \frac{uL}{D}]}{[1 + (\frac{u-v}{u+v})\exp(-uL/D)]}$$

Approximate Solution

$$B(x,t) = B_3(x,t)/B_4(x)$$

where

$$B_3(x,t) = \frac{1}{2}\exp[\frac{(v-u)x}{2D}]\,\mathrm{erfc}\left[\frac{Rx - ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{1}{2} \exp[\frac{(v+u)x}{2D}] \operatorname{erfc}\left[\frac{Rx + ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{(u-v)}{2(u+v)} \exp[\frac{(v+u)x - 2uL}{2D}] \operatorname{erfc}\left[\frac{R(2L-x) - ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{(u+v)}{2(u-v)} \exp[\frac{(v-u)x + 2uL}{2D}] \operatorname{erfc}\left[\frac{R(2L-x) + ut}{2(DRt)^{1/2}}\right]$$

$$- \frac{v^2}{2\mu D} \exp[\frac{vL}{D} - \frac{\mu t}{R}] \operatorname{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$B_4(x) = 1 + (\frac{u-v}{u+v}) \exp(-uL/D)$$

C12. Governing Equation $R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} - \mu c + \gamma$

Initial Condition

$c(x,0) \equiv A(x)$

$$= \frac{\gamma}{\mu} + (C_i - \frac{\gamma}{\mu}) \frac{\exp[\frac{(v-u)x}{2D}] + (\frac{u-v}{u+v}) \exp[\frac{(v+u)x - 2uL}{2D}]}{[\frac{u+v}{2v} - \frac{(u-v)^2}{2v(u+v)} \exp(-uL/D)]}$$

where

$$u = v \left(1 + \frac{4\mu D}{v^2}\right)^{1/2}$$

Note that the initial condition is of the same form as the steady-state solution for the same boundary conditions (case C4).

Boundary Conditions

$$\left.(-D \frac{\partial c}{\partial x} + vc)\right|_{x=0} = \begin{cases} vC_o & 0 < t \leq t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial c}{\partial x}(L,t) = 0$$

Analytical Solution

$$c(x,t) = \begin{cases} A(x) + (C_o - C_i)\, B(x,t) & 0 < t \leq t_o \\ A(x) + (C_o - C_i)\, B(x,t) - C_o\, B(x,t-t_o) & t \geq t_o \end{cases}$$

where A(x) is exactly the initial condition, and where

$$B(x,t) = B_1(x) - B_2(x,t)$$

with

$$B_1(x) = 1 - \sum_{m=1}^{\infty} \frac{E(\beta_m,x)\ \frac{\mu L^2}{D}\ \exp(\frac{vx}{2D})}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{\mu L^2}{D}]}$$

$$B_2(x,t) = \sum_{m=1}^{\infty} \frac{E(\beta_m,x)\ [\beta_m^2 + (\frac{vL}{2D})^2]\ \exp[\frac{vx}{2D} - \frac{\mu t}{R} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}]}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{\mu L^2}{D}]}$$

and

$$E(\beta_m,x) = \frac{\frac{2vL}{D}\ \beta_m [\cos(\frac{\beta_m x}{L}) + \frac{vL}{2D} \sin(\frac{\beta_m x}{L})]}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{vL}{D}]\ [\beta_m^2 + (\frac{vL}{2D})^2]}$$

The eigenvalues β_m are the positive roots of

$$\beta_m \cot(\beta_m) - \frac{\beta_m^2 D}{vL} + \frac{vL}{4D} = 0$$

The term $B_1(x)$, which also appears in the steady-state solution (case C4), converges much slower than the other terms in the series solution. This term, however, can be expressed in an alternative form that is much easier to evaluate:

$$B_1(x) = \frac{\exp[\frac{(v-u)x}{2D}] + (\frac{u-v}{u+v})\ \exp[\frac{(v+u)x - 2uL}{2D}]}{[\frac{u+v}{2v} - \frac{(u-v)^2}{2v(u+v)}\ \exp(-uL/D)]}$$

<u>Approximate Solution</u>

$$B(x,t) = B_3(x,t)/B_4(x,t)$$

where

$$B_3(x,t) = \frac{v}{(v+u)}\ \exp[\frac{(v-u)x}{2D}]\ \mathrm{erfc}\left[\frac{Rx - ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v}{(v-u)}\ \exp[\frac{(v+u)x}{2D}]\ \mathrm{erfc}\left[\frac{Rx + ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v^2}{2\mu D} \exp(\frac{vx}{D} - \frac{\mu t}{R}) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v^2}{2\mu D} [\frac{v(2L-x)}{D} + \frac{v^2 t}{DR} + 3 + \frac{v^2}{\mu D}] \exp(\frac{vL}{D} - \frac{\mu t}{R}) \operatorname{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$- \frac{v^3}{\mu D} (\frac{t}{\pi DR})^{1/2} \exp[\frac{vL}{D} - \frac{\mu t}{R} - \frac{R}{4Dt}(2L-x + \frac{vt}{R})^2]$$

$$+ \frac{v(u-v)}{(u+v)^2} \exp[\frac{(v+u)x - 2uL}{2D}] \operatorname{erfc}\left[\frac{R(2L-x) - ut}{2(DRt)^{1/2}}\right]$$

$$- \frac{v(u+v)}{(u-v)^2} \exp[\frac{(v-u)x + 2uL}{2D}] \operatorname{erfc}\left[\frac{R(2L-x) + ut}{2(DRt)^{1/2}}\right]$$

and

$$B_4(x) = 1 - \frac{(u-v)^2}{(u+v)^2} \exp(-uL/D)$$

C13. Governing Equation $R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} - \mu c + \gamma$

Initial and Boundary Conditions

$c(x,0) = C_i$

$c(0,t) = C_a + C_b e^{-\lambda t}$

$\frac{\partial c}{\partial x} (\infty,t) = 0$

Analytical Solution [see Cleary and Ungs (*1974*) and Marino (*1974*b) for some special cases]

$$c(x,t) = \frac{\gamma}{\mu} + (C_i - \frac{\gamma}{\mu}) A(x,t) + (C_a - \frac{\gamma}{\mu}) B(x,t) + C_b E(x,t)$$

where

$$A(x,t) = \exp(-\mu t/R) \left\{ 1 - \frac{1}{2} \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] - \frac{1}{2} \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right] \right\}$$

$$B(x,t) = \frac{1}{2} \exp[\frac{(v-u)x}{2D}] \operatorname{erfc}\left[\frac{Rx - ut}{2(DRt)^{1/2}}\right] + \frac{1}{2} \exp[\frac{(v+u)x}{2D}] \operatorname{erfc}\left[\frac{Rx + ut}{2(DRt)^{1/2}}\right]$$

$$E(x,t) = e^{-\lambda t} \left\{ \frac{1}{2} \exp[\frac{(v-w)x}{2D}] \operatorname{erfc}\left[\frac{Rx - wt}{2(DRt)^{1/2}}\right] + \frac{1}{2} \exp[\frac{(v+w)x}{2D}] \operatorname{erfc}\left[\frac{Rx + wt}{2(DRt)^{1/2}}\right] \right\}$$

and with

$$u = v\ (1 + \frac{4\mu D}{v^2})^{1/2}$$

$$w = v\ [1 + \frac{4D}{v^2}(\mu - \lambda R)]^{1/2}$$

C14. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} - \mu c + \gamma$$

<u>Initial and Boundary Conditions</u>

$$c(x,0) = C_i$$

$$\left(-D \frac{\partial c}{\partial x} + vc\right)\Big|_{x=0} = v(C_a + C_b e^{-\lambda t})$$

$$\frac{\partial c}{\partial x}(\infty,t) = 0$$

<u>Analytical Solution</u> (see also Lindstrom and Oberhettinger *1975*)

$$c(x,t) =$$

$$\begin{cases} \frac{\gamma}{\mu} + (C_i - \frac{\gamma}{\mu})\ A(x,t) + (C_a - \frac{\gamma}{\mu})\ B(x,t) + C_b\ E(x,t) & (\mu \neq \lambda R) \\ \frac{\gamma}{\mu} + (C_i - C_b - \frac{\gamma}{\mu})\ A(x,t) + (C_a - \frac{\gamma}{\mu})\ B(x,t) + C_b e^{-\lambda t} & (\mu = \lambda R) \end{cases}$$

where

$$A(x,t) = \exp(-\mu t/R) \left\{ 1 - \frac{1}{2} \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] - \left(\frac{v^2 t}{\pi DR}\right)^{1/2} \exp\left[-\frac{(Rx - vt)^2}{4DRt}\right] + \frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right) \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right] \right\}$$

$$B(x,t) = \left(\frac{v}{v+u}\right) \exp\left[\frac{(v-u)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - ut}{2(DRt)^{1/2}}\right] + \left(\frac{v}{v-u}\right) \exp\left[\frac{(v+u)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v^2}{2\mu D} \exp\left(\frac{vx}{D} - \frac{\mu t}{R}\right) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$E(x,t) = e^{-\lambda t}\left\{\left(\frac{v}{v+w}\right) \exp\left[\frac{(v-w)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - wt}{2(DRt)^{1/2}}\right] + \left(\frac{v}{v-w}\right) \exp\left[\frac{(v+w)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + wt}{2(DRt)^{1/2}}\right]\right\}$$

$$+ \frac{v^2}{2D(\mu-\lambda R)} \exp\left(\frac{vx}{D} - \frac{\mu t}{R}\right) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

and

$$u = v \left(1 + \frac{4\mu D}{v^2}\right)^{1/2}$$

$$w = v \left[1 + \frac{4D}{v^2}(\mu - \lambda R)\right]^{1/2}$$

C15. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} - \mu c + \gamma$$

Initial and Boundary Conditions

$$c(x,0) = C_i$$

$$c(0,t) = C_a + C_b e^{-\lambda t}$$

$$\frac{\partial c}{\partial x}(L,t) = 0$$

Analytical Solution

$$c(x,t) = \begin{cases} \frac{\gamma}{\mu} + (C_i - \frac{\gamma}{\mu}) A(x,t) + (C_a - \frac{\gamma}{\mu}) B(x,t) + C_b F(x,t) & (\mu \neq \lambda R) \\ \frac{\gamma}{\mu} + (C_i - C_b - \frac{\gamma}{\mu}) A(x,t) + (C_a - \frac{\gamma}{\mu}) B(x,t) + C_b e^{-\lambda t} & (\mu = \lambda R) \end{cases}$$

where

$$A(x,t) = \sum_{m=1}^{\infty} E(\beta_m,x) \exp[\frac{vx}{2D} - \frac{\mu t}{R} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}]$$

$$B(x,t) = B_1(x) - B_2(x,t)$$

$$B_1(x) = 1 - \sum_{m=1}^{\infty} \frac{E(\beta_m,x) \frac{\mu L^2}{D} \exp(\frac{vx}{2D})}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{\mu L^2}{D}]}$$

$$B_2(x,t) = \sum_{m=1}^{\infty} \frac{E(\beta_m,x) [\beta_m^2 + (\frac{vL}{2D})^2] \exp[\frac{vx}{2D} - \frac{\mu t}{R} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}]}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{\mu L^2}{D}]}$$

$$F(x,t) = e^{-\lambda t}\,[F_1(x) - F_2(x,t)]$$

$$F_1(x) = 1 - \sum_{m=1}^{\infty} \frac{E(\beta_m,x)\,\frac{(\mu - \lambda R)L^2}{D}\,\exp(\frac{vx}{2D})}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{(\mu - \lambda R)L^2}{D}]}$$

$$F_2(x,t) = \sum_{m=1}^{\infty} \frac{E(\beta_m,x)\,[\beta_m^2 + (\frac{vL}{2D})^2]\,\exp[\frac{vx}{2D} - \frac{\mu t}{R} + \lambda t - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}]}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{(\mu - \lambda R)L^2}{D}]}$$

and

$$E(\beta_m,x) = \frac{2\beta_m \sin(\frac{\beta_m x}{L})}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{vL}{2D}]}$$

The eigenvalues β_m are the positive roots of

$$\beta_m \cot(\beta_m) + \frac{vL}{2D} = 0$$

The terms $B_1(x)$ and $F_1(x)$ converge much slower than the other terms in the series solution. Both $B_1(x)$ and $F_1(x)$, however, can be expressed in alternative forms that are much easier to evaluate (case C3):

$$B_1(x) = \frac{\exp[\frac{(v-u)x}{2D}] + (\frac{u-v}{u+v})\,\exp[\frac{(v+u)x - 2uL}{2D}]}{[1 + (\frac{u-v}{u+v})\,\exp(-uL/D)]}$$

$$F_1(x) = \frac{\exp[\frac{(v-w)x}{2D}] + (\frac{w-v}{w+v})\,\exp[\frac{(v+w)x - 2wL}{2D}]}{[1 + (\frac{w-v}{w+v})\,\exp(-wL/D)]}$$

where

$$u = v\,(1 + \frac{4\mu D}{v^2})^{1/2}$$

$$w = v\left[1 + \frac{4D}{v^2}(\mu - \lambda R)\right]^{1/2}$$

<u>Approximate Solution</u>

$$A(x,t) = \exp(-\mu t/R)\left\{1 - \frac{1}{2}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right]\right.$$

$$- \frac{1}{2}\exp(vx/D)\;\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$- \frac{1}{2}\left[2 + \frac{v(2L-x)}{D} + \frac{v^2 t}{DR}\right]\exp(vL/D)\;\mathrm{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$\left. + \left(\frac{v^2 t}{\pi DR}\right)^{1/2}\exp\left[\frac{vL}{D} - \frac{R}{4Dt}\left(2L-x + \frac{vt}{R}\right)^2\right]\right\}$$

$$B(x,t) = B_3(x,t)/B_4(x)$$

where

$$B_3(x,t) = \frac{1}{2}\exp\left[\frac{(v-u)x}{2D}\right]\mathrm{erfc}\left[\frac{Rx - ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{1}{2}\exp\left[\frac{(v+u)x}{2D}\right]\mathrm{erfc}\left[\frac{Rx + ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{(u-v)}{2(u+v)}\exp\left[\frac{(v+u)x - 2uL}{2D}\right]\mathrm{erfc}\left[\frac{R(2L-x) - ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{(u+v)}{2(u-v)}\exp\left[\frac{(v-u)x + 2uL}{2D}\right]\mathrm{erfc}\left[\frac{R(2L-x) + ut}{2(DRt)^{1/2}}\right]$$

$$- \frac{v^2}{2\mu D}\exp\left(\frac{vL}{D} - \frac{\mu t}{R}\right)\mathrm{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$B_4(x) = 1 + (\frac{u-v}{u+v}) \exp(-uL/D)$$

and

$$F(x,t) = e^{-\lambda t} F_3(x,t)/F_4(x)$$

where

$$F_3(x,t) = \frac{1}{2} \exp[\frac{(v-w)x}{2D}] \operatorname{erfc}\left[\frac{Rx - wt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{1}{2} \exp[\frac{(v+w)x}{2D}] \operatorname{erfc}\left[\frac{Rx + wt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{(w-v)}{2(w+v)} \exp[\frac{(v+w)x - 2wL}{2D}] \operatorname{erfc}\left[\frac{R(2L-x) - wt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{(w+v)}{2(w-v)} \exp[\frac{(v-w)x + 2wL}{2D}] \operatorname{erfc}\left[\frac{R(2L-x) + wt}{2(DRt)^{1/2}}\right]$$

$$- \frac{v^2}{2D(\mu - \lambda R)} \exp(\frac{vL}{D} - \frac{\mu t}{R} + \lambda t) \operatorname{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$F_4(x) = 1 + (\frac{w-v}{w+v}) \exp(-wL/D)$$

C16. Governing Equation

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} - \mu c + \gamma$$

Initial and Boundary Conditions

$$c(x,0) = 0$$

$$\left(-D \frac{\partial c}{\partial x} + vc\right)\Big|_{x=0} = v(C_a + C_b\, e^{-\lambda t})$$

$$\frac{\partial c}{\partial x}(L,t) = 0$$

Analytical Solution

$$c(x,t) =$$

$$\begin{cases} \frac{\gamma}{\mu} + (C_i - \frac{\gamma}{\mu})\, A(x,t) + (C_a - \frac{\gamma}{\mu})\, B(x,t) + C_b\, F(x,t) & (\mu \neq \lambda R) \\ \frac{\gamma}{\mu} + (C_i - C_b - \frac{\gamma}{\mu})\, A(x,t) + (C_a - \frac{\gamma}{\mu})\, B(x,t) + C_b e^{-\lambda t} & (\mu = \lambda R) \end{cases}$$

where

$$A(x,t) = \sum_{m=1}^{\infty} E(\beta_m, x)\, \exp\left[\frac{vx}{2D} - \frac{\mu t}{R} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}\right]$$

$$B(x,t) = B_1(x) - B_2(x,t)$$

$$B_1(x) = 1 - \sum_{m=1}^{\infty} \frac{E(\beta_m, x)\, \frac{\mu L^2}{D}\, \exp(\frac{vx}{2D})}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{\mu L^2}{D}]}$$

$$B_2(x,t) = \sum_{m=1}^{\infty} \frac{E(\beta_m, x)\, [\beta_m^2 + (\frac{vL}{2D})^2]\, \exp[\frac{vx}{2D} - \frac{\mu t}{R} - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}]}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{\mu L^2}{D}]}$$

$$F(x,t) = e^{-\lambda t}[F_1(x) - F_2(x,t)]$$

$$F_1(x) = 1 - \sum_{m=1}^{\infty} \frac{E(\beta_m,x)\ \frac{(\mu - \lambda R)L^2}{D}\ \exp(\frac{vx}{2D})}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{(\mu - \lambda R)L^2}{D}}$$

$$F_2(x,t) = \sum_{m=1}^{\infty} \frac{E(\beta_m,x)\ [\beta_m^2 + (\frac{vL}{2D})^2]\ \exp[\frac{vx}{2D} - \frac{\mu t}{R} + \lambda t - \frac{v^2 t}{4DR} - \frac{\beta_m^2 Dt}{L^2 R}]}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{(\mu - \lambda R)L^2}{D}]}$$

and

$$E(\beta_m,x) = \frac{\frac{2vL}{D}\ \beta_m\ [\beta_m \cos(\frac{\beta_m x}{L}) + (\frac{vL}{2D}) \sin(\frac{\beta_m x}{L})]}{[\beta_m^2 + (\frac{vL}{2D})^2 + \frac{vL}{D}]\ [\beta_m^2 + (\frac{vL}{2D})^2]}$$

The eigenvalues β_m are the positive roots of

$$\beta_m \cot(\beta_m) - \frac{\beta_m^2 D}{vL} - \frac{vL}{4D} = 0$$

The terms $B_1(x)$ and $F_1(x)$ converge much slower than the other terms in the series solution. Both $B_1(x)$ and $F_1(x)$, however, can be expressed in alternative forms that are much easier to evaluate (case C4):

$$B_1(x) = \frac{\exp[\frac{(v-u)x}{2D}] + (\frac{u-v}{u+v}) \exp[\frac{(v+u)x - 2uL}{2D}]}{[\frac{u+v}{2v} - \frac{(u-v)^2}{2v(u+v)} \exp(-uL/D)]}$$

$$F_1(x) = \frac{\exp \frac{(v-w)x}{2D} + (\frac{w-v}{w+v}) \exp[\frac{(v+w)x - 2wL}{2D}]}{[(\frac{w+v}{2v}) - \frac{(w-v)^2}{2v(w+v)} \exp(-wL/D)]}$$

where

$$u = v\left(1 + \frac{4\mu D}{v^2}\right)^{1/2}$$

$$w = v\left[1 + \frac{4D}{v^2}(\mu - \lambda R)\right]^{1/2}$$

Approximate Solution

$$A(x,t) = \exp(-\mu t/R)\Bigg\{1 - \frac{1}{2}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] - \left(\frac{v^2 t}{\pi DR}\right)^{1/2}\exp\left[-\frac{(Rx - vt)^2}{4DRt}\right]$$

$$+ \frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right)\exp(vx/D)\,\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$- \left(\frac{4v^2 t}{\pi DR}\right)^{1/2}\left[1 + \frac{v}{4D}\left(2L - x + \frac{vt}{R}\right)\right]\exp\left[\frac{vL}{D} - \frac{R}{4Dt}\left(2L - x + \frac{vt}{R}\right)^2\right]$$

$$+ \frac{v}{D}\left[2L - x + \frac{3vt}{2R} + \frac{v}{4D}\left(2L - x + \frac{vt}{R}\right)^2\right]\exp(vL/D)\,\mathrm{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]\Bigg\}$$

$$B(x,t) = B_3(x,t)/B_4(x,t)$$

where

$$B_3(x,t) = \frac{v}{(v+u)}\exp\left[\frac{(v-u)x}{2D}\right]\mathrm{erfc}\left[\frac{Rx - ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v}{(v-u)}\exp\left[\frac{(v+u)x}{2D}\right]\mathrm{erfc}\left[\frac{Rx + ut}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v^2}{2\mu D}\exp\left(\frac{vx}{D} - \frac{\mu t}{R}\right)\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v^2}{2\mu D}\left[\frac{v(2L-x)}{D} + \frac{v^2 t}{DR} + 3 + \frac{v^2}{\mu D}\right]\exp\left(\frac{vL}{D} - \frac{\mu t}{R}\right)\mathrm{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$- \frac{v^3}{\mu D} \left(\frac{t}{\pi DR}\right)^{1/2} \exp\left[\frac{vL}{D} - \frac{\mu t}{R} - \frac{R}{4Dt}\left(2L-x + \frac{vt}{R}\right)^2\right]$$

$$+ \frac{v(u-v)}{(u+v)^2} \exp\left[\frac{(v+u)x - 2uL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) - ut}{2(DRt)^{1/2}}\right]$$

$$- \frac{v(u+v)}{(u-v)^2} \exp\left[\frac{(v-u)x + 2uL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) + ut}{2(DRt)^{1/2}}\right]$$

$$B_4(x) = 1 - \frac{(u-v)^2}{(u+v)^2} \exp(-uL/D)$$

and

$$F(x,t) = e^{-\lambda t} F_3(x,t)/F_4(x)$$

where

$$F_3(x,t) = \left(\frac{v}{v+w}\right) \exp\left[\frac{(v-w)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - wt}{2(DRt)^{1/2}}\right]$$

$$+ \left(\frac{v}{v-w}\right) \exp\left[\frac{(v+w)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + wt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v^2}{2D(\mu-\lambda R)} \exp\left(\frac{vx}{D} - \frac{\mu t}{R} + \lambda t\right) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]$$

$$+ \frac{v^2}{2D(\mu-\lambda R)} \left[\frac{v(2L-x)}{D} + \frac{v^2 t}{DR} + 3 + \frac{v^2}{D(\mu-\lambda R)}\right]$$

$$\exp\left(\frac{vL}{D} - \frac{\mu t}{R} + \lambda t\right) \operatorname{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]$$

$$- \frac{v^3}{D(\mu-\lambda R)} \left(\frac{t}{\pi DR}\right)^{1/2} \exp\left[\frac{vL}{D} - \frac{\mu t}{R} + \lambda t - \frac{R}{4Dt}\left(2L-x + \frac{vt}{R}\right)^2\right]$$

$$+ \frac{v(w-v)}{(w+v)^2} \exp\left[\frac{(v+w)x - 2wL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) - wt}{2(DRt)^{1/2}}\right]$$

$$- \frac{v(w+v)}{(w-v)^2} \exp\left[\frac{(v-w)x + 2wL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) + wt}{2(DRt)^{1/2}}\right]$$

$$F_4(x) = 1 - \frac{(w-v)^2}{(w+v)^2} \exp(-wL/D)$$

5. EFFECT OF BOUNDARY CONDITIONS

In this section we will present several calculated solute distributions as a function of distance and time. Special attention will be given to the effects of the applied upper and lower boundary conditions. The results are generalized by making use of the following dimensionless variables

$$P = vL/D \qquad T = vt/L \qquad z = x/L \qquad [14]$$

where P is the column Peclet number, T is the number of displaced pore volumes, and z is the reduced distance. To make the solutions for a semi-infinite system applicable to a finite profile of length L (for example, a laboratory soil column), the reduced distance cannot exceed one ($0 \leqslant x \leqslant L$).

Figure 1 shows calculated distributions obtained with the solutions of cases A1 (first-type boundary condition at $x = 0$; semi-infinite profile), A2 (third-type boundary condition; semi-infinite profile), A3 (first-type boundary condition; finite profile), and A4 (third-type boundary condition; finite profile). Results are given for P-values of 5 and 20, and at times equivalent to displaced pore volumes of 0.25 and 1.0. The retardation factor (R) is assumed to be one; by replacing T by T/R, the curves in figure 1 also hold for values of R other than one. Furthermore, the curves are for no production and decay ($\gamma = \mu = 0$), for an initial concentration (C_i) of zero, and for a continuous input concentration (C_o) of one.

A considerable effect of the upper boundary condition on the results is apparent at a Peclet number of 5. The curves for a first-type boundary condition (cases A1 and A3) are much higher than those for a third-type boundary condition (A2, A4) throughout the entire profile. The curves for a semi-infinite system (A1, A2), furthermore, are very similar to those for a finite system (A3, A4) at relatively small times ($T < 0.25$ in fig. 1). This similarity occurs when the solute fronts are still not influenced by the lower boundary. Large differences between the solutions for a finite and semi-infinite system, however, are present at later times. These differences are greatest after about one pore volume. When P increases from 5 to 20, the differences between the various solutions become much smaller. Note that for $P = 20$ the solutions for a finite and semi-infinite system deviate from each other only in a very small region near the lower boundary.

From a large number of comparisons we found that the solution for a finite system can be approximated with an accuracy of at

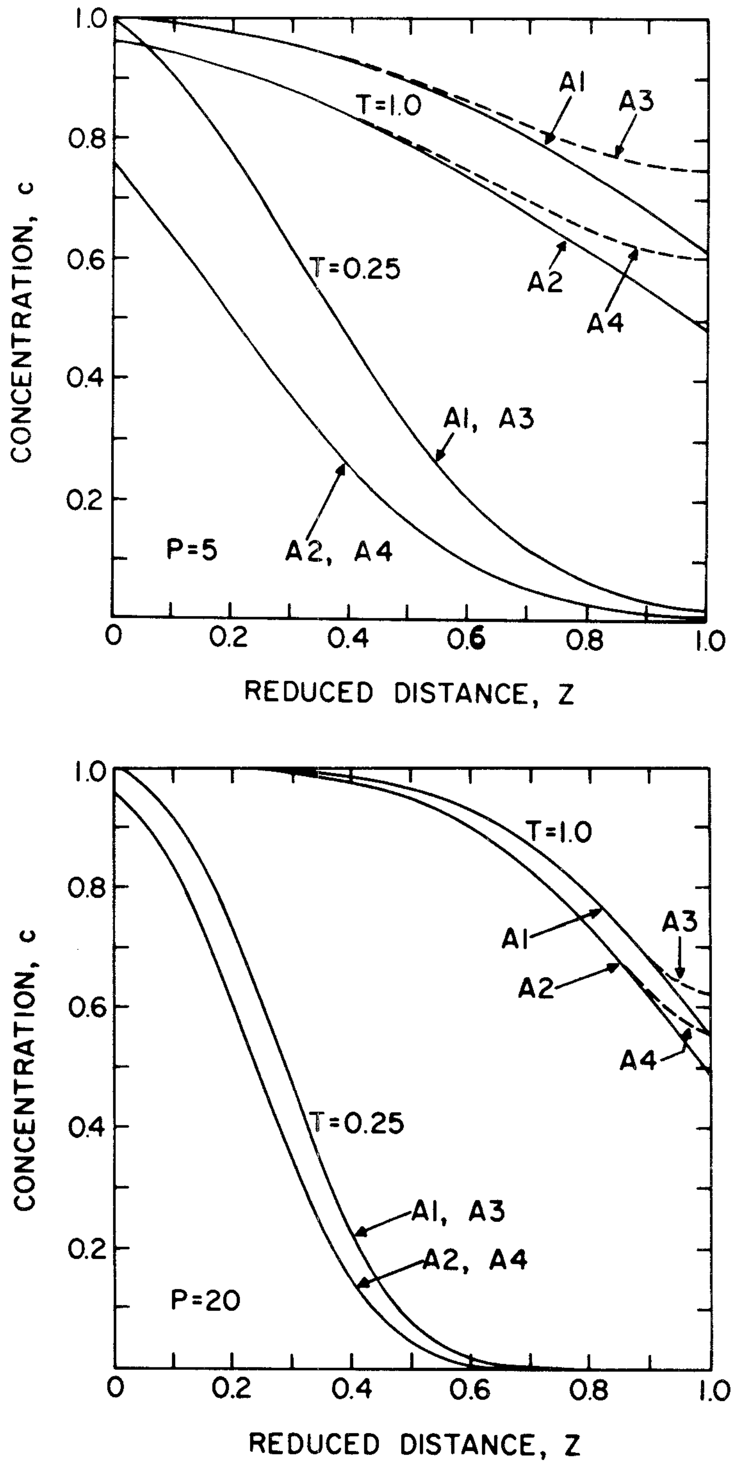

Figure 1. Calculated concentration distributions for R=1 and P-values of 5 and 20, respectively. The curves were obtained with the analytical solutions of cases A1, A2, A3, and A4.

least four significant places by solutions for a semi-infinite system as long as z is restricted to

$$0 \leq z \leq .9 - 8/P. \qquad [15]$$

This empirical rule, which holds for all values of T, applies also for cases where production or decay terms are present. For relatively small values of T (for example, for T less than 0.25 in fig. 1), [15] could be expanded to a much larger part of the profile.

Except for the region close to the column entrance, the largest differences between the four solutions occur at the lower boundary after about one pore volume. Figure 2 shows the effect of P on the lower boundary concentration at T = 1 for the four analytical solutions. The curves diverge considerably from each other at the lower Peclet numbers. The curves for A1 and A4 approach each other slowly when P increases; at a Peclet number of 10, the difference is only 0.05 unit. The curve for A2, although always less than 0.5, converges to 0.5 rather quickly; it reaches a value of 0.493 at P = 10.

Differences among the various analytical solutions, such as those shown in figure 2, are important. Estimates of the coefficients P and R in the transport equation are often obtained by fitting one of the analytical solutions (A1 to A4) to observed column effluent data (van Genuchten *1980*). This procedure assumes that the exit concentration can be equated to the concentration at the lower boundary.

Although considerable differences between the analytical solutions are present, even at Peclet numbers as high as 100 to 200, the significance of these differences are somewhat misleading when judged from figure 2 alone. This is because of the increasingly steeper slope of the exit concentration when plotted against T. This effect is shown in figure 3, where effluent curves are given for Peclet numbers of 5, 20, and 60. Figure 3c shows that only a small displacement is needed to let all solutions converge to the same curve (P = 60). The maximum differences between the curves in figures 3b and 3c, furthermore, are roughly of the same order of magnitude as the experimental errors one may expect in carefully obtained effluent curves. It seems likely, therefore, that the effects of the imposed mathematical boundary conditons can be neglected when P reaches values of about 20 or 30.

Two additional observations follow from figure 3. First, the effluent curves for cases A1 and A4 are very close when P is about 5 or higher. This property was demonstrated earlier by

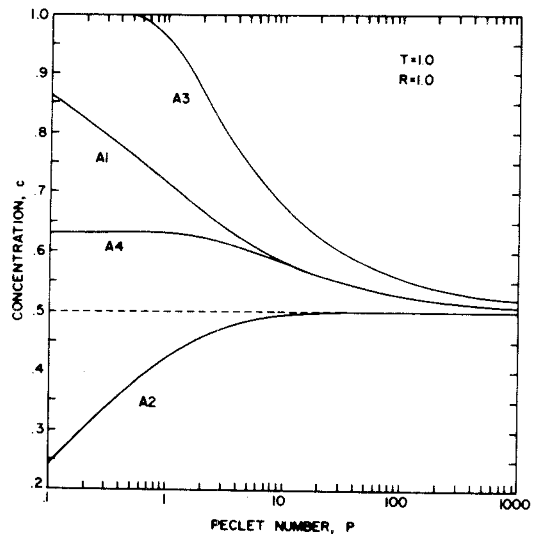

Figure 2. Effect of P on the concentration at x = L and for T = 1. The curves were obtained with the analytical solutions of cases A1, A2, A3, and A4.

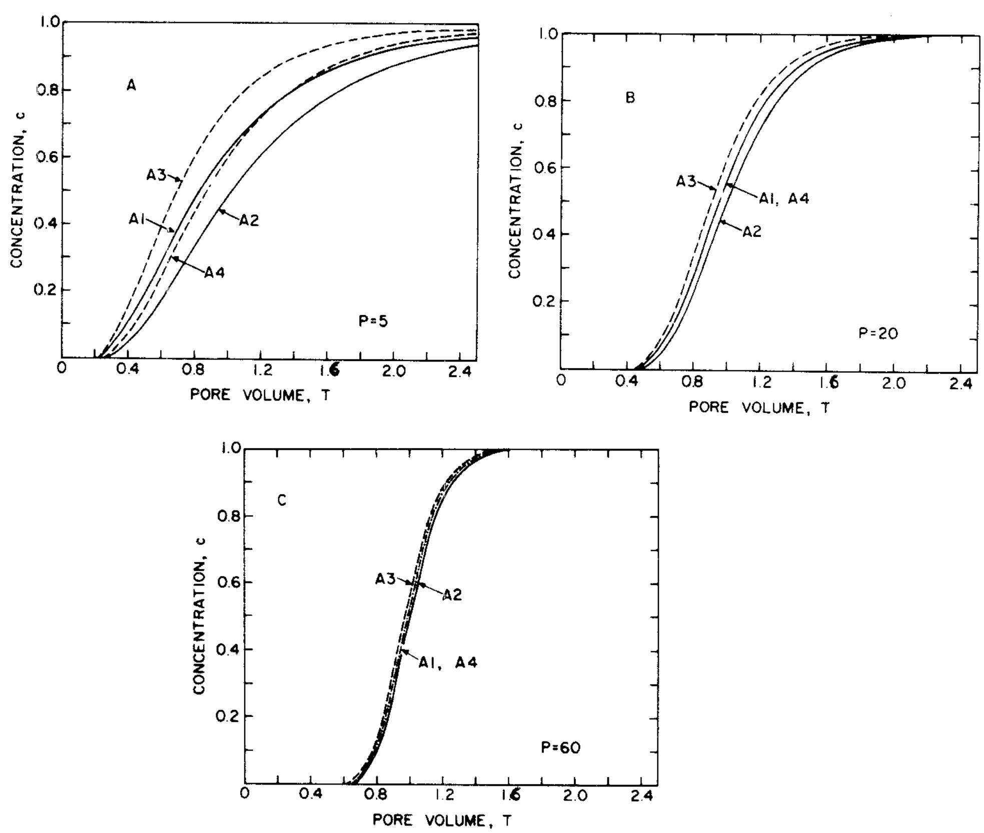

Figure 3. Effect of P on calculated effluent curves for cases A1, A2, A3, and A4.

Parlange and Starr (*1975*). The errors introduced by approximating the solution of A4 by the much simpler solution of A1 are about the same as the differences between the curves A1 and A4 in figure 2. Second, the curves for A1 in figure 3 are located exactly between those for A2 and A3. In equation form this can be expressed as

$$c_{A3} = 2c_{A1} - c_{A2} \qquad (x=L) \qquad [16]$$

where the subscripts A1, A2, and A3 refer to the appropriate analytical solutions. This last property, which is extremely accurate for values of P that are not too small, follows directly from the approximate solution of case A3. Similar relations apply for all approximate solutions for a finite system and a first-type boundary condition at x = 0 (that is, also for nonzero values of λ, μ, and γ). For example, for case C7 one has

$$c_{C7} = 2c_{C5} - c_{C6}. \qquad (x=L) \qquad [17]$$

The above discussion of the boundary effects is restricted to cases where the production and decay terms are zero. Similar effects of the boundary conditions can also be demonstrated when either γ, μ, or both are nonzero. Only a few comments for these cases will be given here. The effects of the boundary conditions are generally more pronounced for the special case of zero-order production only ($\gamma \neq 0$, $\mu = 0$). This is shown in figure 4 where the steady-state solutions of cases B1 to B4 are plotted for two values of the column Peclet number. Results are given for $C_o = 1$ and a value of one for the dimensionless rate term

$$\bar{\gamma} = \gamma L/v. \qquad [18]$$

The differences between the four solutions are considerable, especially when P equals 5. Note that the solution for case B1 is independent of P.

The effects of the boundary conditions are generally less significant when, in addition to zero-order production, the chemical is also subject to first-order decay. Figure 5 shows the steady-state solutions of cases C1 to C4, for two values of $\bar{\gamma}$, and for a value of one for the dimensionless decay constant

$$\bar{\mu} = \mu L/v. \qquad [19]$$

The curves for the two values of $\bar{\gamma}$ are, in this particular example, symmetric with respect to the line c = 1. Note that,

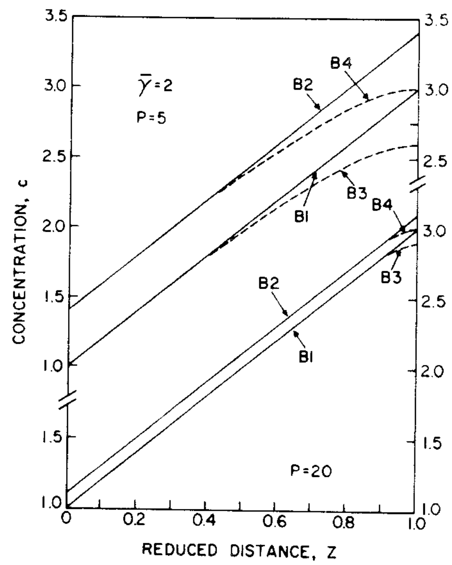

Figure 4. Effect of P on steady-state concentration distributions for cases B1, B2, B3, and B4.

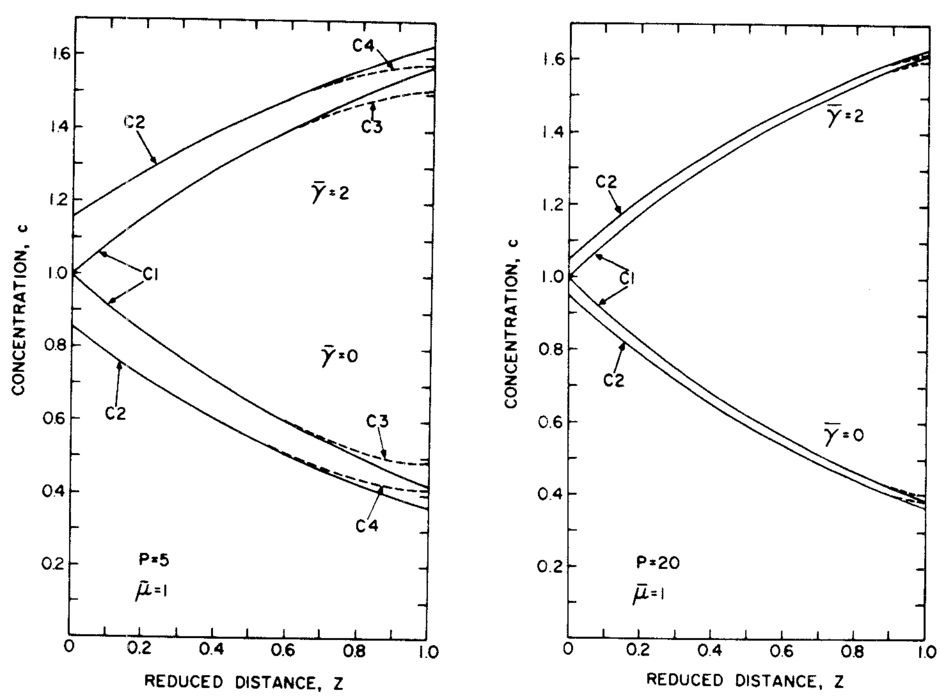

Figure 5. Effect of P on steady-state concentration distributions for cases C1, C2, C3, and C4.

at a Peclet number of 20, the finite and semi-infinite solutions are essentially the same over the region $0 < z < 0.95$. The effects of the boundary conditions are generally more pronounced when the ratio γ/μ increases; the effects are relatively small when $\gamma = 0$ and μ is large.

6. NOTATION

Symbol	Definition
c	Solution concentration.
c_{A1}, c_{A2}, c_{A3}	Effluent concentrations based on the solutions of cases A1, A2 and A3, respectively.
c_{C5}, c_{C6}, c_{C7}	Effluent concentrations based on the solutions of cases C5, C6, and C7, respectively.
C_1, C_2	Constants in several initial conditions (table 1).
C_a, C_b	Constants in several boundary conditions (table 1).
C_i	Initial concentration (table 1).
C_o	Input concentration (table 1).
D	Dispersion coefficient.
$f(x)$	General initial condition.
$g(t)$	General input concentration.
k	Distribution constant.
L	Column length.
P	Column Peclet number ($P = vL/D$).
q	Volumetric flux.
R	Retardation factor ($R = 1 + \rho k/\theta$).
S	Adsorbed concentration.
t	Time.
t_o	Duration of solute pulse (table 1).

T	Pore volume ($T = vt/L$).
u	$u = (v^2 + 4\mu D)^{1/2}$.
v	Pore-water velocity.
w	$w = [v^2 + 4D(\mu-\lambda R]^{1/2}$.
x	Distance.
x_1	Constant in several initial conditions (table 1).
y	$y = (v^2 - 4\lambda DR)^{1/2}$.
z	Reduced distance ($z = x/L$).
α	Decay constant in several initial conditions (table 1).
β_m	m-th eigenvalue.
γ	General zero-order rate coefficient for production.
γ_s	Zero-order solid phase rate coefficient for production.
γ_w	Zero-order liquid phase rate coefficient for production.
$\bar{\gamma}$	Dimensionless zero-order rate coefficient ($\bar{\gamma} = \gamma L/v$).
θ	Volumetric moisture content.
λ	Decay constant in several boundary conditions (table 1).
μ	General first-order rate coefficient for decay.
μ_s	First-order solid phase rate coefficient for decay.
μ_w	First-order liquid phase rate coefficient for decay.
$\bar{\mu}$	Dimensionless first-order rate coefficient ($\bar{\mu} = \mu L/v$).
ρ	Bulk density

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APPENDIX A.--TABLE OF LAPLACE TRANSFORMS

$$f(s) = \int_0^\infty e^{-st} F(t)\, dt$$

The following abbreviations are used in the table:

$$A = \frac{1}{\sqrt{\pi t}} \exp(-\frac{x^2}{4t})$$

$$B = \text{erfc}(\frac{x}{2\sqrt{t}})$$

$$C = \exp(a^2 t - ax)\ \text{erfc}(\frac{x}{2\sqrt{t}} - a\sqrt{t})$$

$$D = \exp(a^2 t + ax)\ \text{erfc}(\frac{x}{2\sqrt{t}} + a\sqrt{t})$$

f(s)	F(t)
$e^{-x\sqrt{s}}$	$\frac{x}{2t} A$
$\frac{e^{-x\sqrt{s}}}{\sqrt{s}}$	A
$\frac{e^{-x\sqrt{s}}}{s}$	B
$\frac{e^{-x\sqrt{s}}}{s\sqrt{s}}$	$2t\ A - x\ B$
$\frac{e^{-x\sqrt{s}}}{s^2}$	$\frac{1}{2} (x^2 + 2t)\ B - xt\ A$

APPENDIX A.--Table of Laplace Transforms--Continued

f(s)	F(t)
$\frac{e^{-x\sqrt{s}}}{s^{1+n/2}}$	$(4t)^{n/2}\ i^n\mathrm{erfc}(\frac{x}{2\sqrt{t}})$ (n=0,1,2,...)
$\frac{\sqrt{s}\ e^{-x\sqrt{s}}}{s-a^2}$	$A + \frac{a}{2}(C - D)$
$\frac{e^{-x\sqrt{s}}}{s-a^2}$	$\frac{1}{2}(C + D)$
$\frac{e^{-x\sqrt{s}}}{\sqrt{s}(s-a^2)}$	$\frac{1}{2a}(C - D)$
$\frac{\sqrt{s}\ e^{-x\sqrt{s}}}{(s-a^2)^2}$	$t\ A + \frac{1}{4a}(1 - ax + 2a^2t)\ C - \frac{1}{4a}(1 + ax + 2a^2t)\ D$
$\frac{e^{-x\sqrt{s}}}{(s-a^2)^2}$	$\frac{1}{4a}(2at - x)\ C + \frac{1}{4a}(2at + x)\ D$
$\frac{e^{-x\sqrt{s}}}{\sqrt{s}(s-a^2)^2}$	$\frac{t}{a^2}A - \frac{1}{4a^3}(1 + ax - 2a^2t)\ C + \frac{1}{4a^3}(1 - ax - 2a^2t)\ D$
$\frac{\sqrt{s}\ e^{-x\sqrt{s}}}{a+\sqrt{s}}$	$(\frac{x}{2t} - a)\ A + a^2\ D$
$\frac{e^{-x\sqrt{s}}}{a+\sqrt{s}}$	$A - a\ D$

APPENDIX A.--Table of Laplace Transforms--Continued

f(s)	F(t)
$\frac{e^{-x\sqrt{s}}}{\sqrt{s}(a+\sqrt{s})}$	D
$\frac{e^{-x\sqrt{s}}}{s(a+\sqrt{s})}$	$\frac{1}{a}(B - D)$
$\frac{e^{-x\sqrt{s}}}{s\sqrt{s}(a+\sqrt{s})}$	$\frac{2t}{a} A - \frac{1}{a^2}(1 + ax) B + \frac{1}{a^2} D$
$\frac{e^{-x\sqrt{s}}}{s^2(a+\sqrt{s})}$	$\frac{1}{a^3}(1 + ax + a^2t + \frac{1}{2} a^2x^2) B$ $- \frac{1}{a^3} D - \frac{t}{a^2}(2 + ax) A$
$\frac{e^{-x\sqrt{s}}}{s^{(n+1)/2}(a+\sqrt{s})}$	$\frac{1}{(-a)^n}\left[D - \sum_{r=0}^{n-1} (-2a\sqrt{t})^r \, i^r\mathrm{erfc}(\frac{x}{2\sqrt{t}})\right]$
$\frac{\sqrt{s}\, e^{-x\sqrt{s}}}{(s-a^2)(a+\sqrt{s})}$	$\frac{1}{4} C + \frac{1}{4}(3 + 2ax + 4a^2t) D - at A$
$\frac{e^{-x\sqrt{s}}}{(s-a^2)(a+\sqrt{s})}$	$t A + \frac{1}{4a} C - \frac{1}{4a}(1 + 2ax + 4a^2t) D$
$\frac{e^{-x\sqrt{s}}}{\sqrt{s}(s-a^2)(a+\sqrt{s})}$	$\frac{1}{4a^2} C + \frac{1}{4a^2}(-1 + 2ax + 4a^2t) D - \frac{t}{a} A$
$\frac{e^{-x\sqrt{s}}}{s(s-a^2)(a+\sqrt{s})}$	$\frac{1}{4a^3} C + \frac{1}{4a^3}(3 - 2ax - 4a^2t) D$ $- \frac{1}{a^3} B + \frac{t}{a^2} A$

APPENDIX A.--Table of Laplace Transforms--Continued

f(s)	F(t)
$\frac{e^{-x\sqrt{s}}}{(s-a^2)^2(a+\sqrt{s})}$	$\frac{t}{4a^2}(1+ax+2a^2t)\ A + \frac{1}{16a^3}(4a^2t-2ax-1)\ C - \frac{1}{16a^3}[4a^2t-1+2a^2(x+2at)^2]\ D$
$\frac{\sqrt{s}\ e^{-x\sqrt{s}}}{(a+\sqrt{s})^2}$	$(1+2a^2t)\ A - a(2+ax+2a^2t)\ D$
$\frac{e^{-x\sqrt{s}}}{(a+\sqrt{s})^2}$	$(1+ax+2a^2t)\ D - 2at\ A$
$\frac{e^{-x\sqrt{s}}}{\sqrt{s}(a+\sqrt{s})^2}$	$2t\ A - (x+2at)\ D$
$\frac{e^{-x\sqrt{s}}}{s(a+\sqrt{s})^2}$	$\frac{1}{a^2}(-1+ax+2a^2t)\ D + \frac{1}{a^2}\ B - \frac{2t}{a}\ A$
$\frac{e^{-x\sqrt{s}}}{s\sqrt{s}(a+\sqrt{s})^2}$	$\frac{4t}{a^2}\ A - \frac{1}{a^3}(2+ax)\ B - \frac{1}{a^3}(-2+ax+2a^2t)\ D$
$\frac{e^{-x\sqrt{s}}}{s^2(a+\sqrt{s})^2}$	$\frac{1}{a^4}(3+2ax+a^2t+\frac{1}{2}a^2x^2)\ B + \frac{1}{a^4}(-3+ax+2a^2t)\ D - \frac{1}{a^3}(6+ax)t\ A$

APPENDIX A.--Table of Laplace Transforms--Continued

f(s)	F(t)
$\frac{\sqrt{s}\ e^{-x\sqrt{s}}}{(s-a^2)(a+\sqrt{s})^2}$	$\frac{t}{2}(3 + ax + 2a^2t)\ A + \frac{1}{8a}\ C$ $- \frac{1}{8a}[1 + 6ax + 16\ a^2t + 2a^2(x + 2at)^2]\ D$
$\frac{e^{-x\sqrt{s}}}{(s-a^2)(a+\sqrt{s})^2}$	$\frac{1}{8a^2}\ C - \frac{t}{2a}(1 + ax + 2a^2t)\ A$ $+ \frac{1}{8a^2}[-1 + 2ax + 8a^2t + 2a^2(x + 2at)^2]\ D$
$\frac{e^{-x\sqrt{s}}}{\sqrt{s}(s-a^2)(a+\sqrt{s})^2}$	$\frac{t}{2a^2}(-1 + ax + 2a^2t)\ A + \frac{1}{8a^3}\ C$ $- \frac{1}{8a^3}[1 - 2ax + 2a^2(x + 2at)^2]\ D$
$\frac{e^{-x\sqrt{s}}}{(s-a^2)^2(a+\sqrt{s})^2}$	$\frac{1}{16a^4}[1 + a(4a^2t - 1)(x + 2at)$ $+ \frac{4}{3}a^3(x + 2at)^3]\ D$ $- \frac{1}{16a^4}(1 + ax - 2a^2t)\ C$ $- \frac{t}{12a^3}[-3 + 4a^2t + a^2(x + 2at)^2]\ A$
$\frac{\sqrt{s}\ e^{-x\sqrt{s}}}{(a+\sqrt{s})^3}$	$[1 + 2ax + 5a^2t + \frac{a^2}{2}(x + 2at)^2]\ D$ $- at(4 + ax + 2a^2t)\ A$
$\frac{e^{-x\sqrt{s}}}{(a+\sqrt{s})^3}$	$t(2 + ax + 2a^2t)\ A$ $- [x + 3at + \frac{a}{2}(x + 2at)^2]\ D$

APPENDIX A.--Table of Laplace Transforms--Continued

f(s)	F(t)
$\frac{e^{-x\sqrt{s}}}{\sqrt{s}(a+\sqrt{s})^3}$	$[t + \frac{1}{2}(x + 2at)^2]\ D - t(x + 2at)\ A$
$\frac{e^{-x\sqrt{s}}}{(s-a^2)(a+\sqrt{s})^3}$	$\frac{t}{12a^2}[-3 + 3ax + 14a^2t + 2a^2(x + 2at)^2]\ A$ $+ \frac{1}{16a^3}[C + (2ax - 1)\ D]$ $- \frac{1}{24a}[3(x + 2at)(x + 6at) + 2a(x + 2at)^3]\ D$
$\frac{\sqrt{s}\ e^{-x\sqrt{s}}}{(a+\sqrt{s})^4}$	$t[2 + 2ax + \frac{16}{3}a^2t + \frac{a^2}{3}(x + 2at)^2]\ A$ $- [x + at + a(x + 2at)(x + 3at)$ $+ \frac{a^2}{3}(x + 2at)^3]\ D$
$\frac{e^{-x\sqrt{s}}}{(a+\sqrt{s})^4}$	$[t + \frac{1}{2}(x + 2at)(x + 4at) + \frac{a}{6}(x + 2at)^3]\ D$ $- \frac{t}{3}[3x + 10\ at + a(x + 2at)^2]\ A$
$\frac{e^{-x\sqrt{s}}}{\sqrt{s}(a+\sqrt{s})^4}$	$\frac{t}{3}[4t + (x + 2at)^2]\ A$ $- [t(x + 2at) + \frac{1}{6}(x + 2at)^2]\ D$
$\frac{e^{-x\sqrt{s}}}{(s-a^2)(b+\sqrt{s})}$	$\frac{1}{2(a+b)}\ C - \frac{1}{2(a-b)}\ D$ $+ \frac{b}{a^2 - b^2}\exp(b^2t + bx)\ \mathrm{erfc}(\frac{x}{2\sqrt{t}} + b\sqrt{t})$

APPENDIX B.--SELECTED COMPUTER PROGRAMS

This appendix contains a series of tables listing user-oriented computer programs of several key analytical solutions of the one-dimensional convective-dispersive transport equation. Each program is augmented with sample input data and associated listings of the computer printout. The sample programs considered are those for cases A1 (together with A2), A3, B14, and C8. A numerical computer solution (N1) is also provided. This solution may be used for those cases where no analytical solution is available.

Table 2 (page 111) lists the most significant variables in the computer programs. The names of similar variables in different programs have been kept the same whenever possible. Table 3 lists the sample input data used for the five computer programs. A listing of the function EXF, which is common to all programs except N1, is given separately in table 4. This function will be discussed below. Listings of the programs themselves, together with the computer output, are given in tables 5 and 6 for case A1, tables 7 and 8 for case A3, tables 9 and 10 for case B14, tables 11 and 12 for case C8, and tables 13 and 14 for case N1 (the numerical solution).

The function EXF(A,B), which appears in all programs except N1, is listed in table 4. This function defines the product of the exponential function (exp) and the complementary error function (erfc) as follows

$$\mathrm{EXF}(A,B) = \exp(A)\ \mathrm{erfc}(B) \qquad [B1]$$

where

$$\mathrm{erfc}(B) = \frac{2}{\sqrt{\pi}} \int_B^\infty \exp(-\tau^2)\ d\tau. \qquad [B2]$$

Two different approximations are used for EXF(A,B). For $0 \leqslant B \leqslant 3$ (see also equation [7.1.26] of Abramowitz and Stegun *1970*):

$$\mathrm{EXF}(A,B) \simeq \exp(A - B^2)(a_1\tau + a_2\tau^2 + a_3\tau^3 + a_4\tau^4 + a_5\tau^5) \qquad [B3]$$

where

$$\tau = \frac{1}{1 + 0.3275911\ B} \qquad [B4]$$

$$a_1 = .2548296 \qquad a_2 = -.2844967$$
$$a_3 = 1.421414 \qquad a_4 = -1.453152$$
$$a_5 = 1.061405 \qquad [B5]$$

and for $B > 3$ (see also equation [7.1.14] of Abramowitz and Stegun *1970*):

$$EXF(A,B) \simeq \frac{1}{\sqrt{\pi}} \exp(A - B^2)/(B + 0.5/(B + 1./(B + 1.5/(B + 2./(B + 2.5/(B + 1.)))))). \qquad [B6]$$

For negative values of B, the following additional relation is used:

$$EXF(A,B) = 2 \exp(A) - EXF(A,-B). \qquad [B7]$$

The function EXF(A,B) can not be used for very small or very large values of its arguments A, B. The function returns zero for the following two conditions:

$$|A| > 170,\ B < 0 \quad \text{or} \quad |A - B^2| > 170,\ B > 0 \qquad [B8]$$

The computer programs for the analytical solutions are all written in double precision FORTRAN IV; they produce answers that have an accuracy of at least four significant digits. Initially, some problems were encountered with an accurate evaluation of the approximate solutions for the finite systems, especially those that are applicable to flux-type soil surface boundary conditions (cases A4, C8). These approximate solutions require the addition and substraction of very large numbers, leading to large roundoff errors and an overall accuracy of at most three significant places when $P > 100$. The following procedure, first suggested by Brenner (*1962*), was used to derive alternative and more easily evaluated forms of the approximate solutions.

As an example, consider the approximate solution C_{A4} of case A4. This solution can be written in the form

$$c_{A4} = c_{A2} + G(x,t) \qquad [B9]$$

where c_{A2} is the analytical solution of case A2 and where G(x,t) is given by

$$G(x,t) = \left(\frac{4v^2t}{\pi DR}\right)^{1/2} \left[1 + \frac{v}{4D}\left(2L-x + \frac{vt}{R}\right)\right] \exp\left[\frac{vL}{D} - \frac{R}{4Dt}\left(2L-x + \frac{vt}{R}\right)^2\right]$$

$$- \frac{v}{D} [2L-x + \frac{3vt}{2R} + \frac{v}{4D}(2L-x + \frac{vt}{R})^2].$$

$$\exp(vL/D) \ \mathrm{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right] \qquad [B10]$$

The approximate solution is used only for relatively large values of the argument in the erfc-function of [B10]. A suitable asymptotic expansion for erfc is therefore (equation 7.1.23 of Abramowitz and Stegun *1970*):

$$\mathrm{erfc}(B) = \frac{\exp(-B^2)}{B\sqrt{\pi}} \left\{ 1 + \sum_{m=1}^{\infty} \frac{(-1)^m \ [1.3....(2m-1)]}{2^m \ B^{2m}} \right\} \qquad [B11]$$

Substituting [B11] into [B10] and combining appropriate terms allows several of the lead terms in the series to be cancelled. Additional simplification leads to the new form

$$G(x,t) = \left(\frac{4v^2t}{\pi DR}\right)^{1/2} \exp\left[\frac{vL}{D} - \frac{R}{4Dt} (2L-x + \frac{vt}{R})^2 \right].$$

$$\sum_{m=1}^{\infty} \frac{(-1)^{m+1}[1.3....(2m-1)] \left(\frac{2Dt}{R}\right)^m [2L-x - \frac{(m-1)vt}{R}]}{(2L-x + \frac{vt}{R})^{2m+1}} \qquad [B12]$$

This series expansion converges rapidly; at most five terms of the series are needed to generate answers that have an accuracy of 4 significant digits. An important advantage of [B12] is that the expression now can be evaluated easily in single precision arithmetic without affecting the four-place accuracy. However, the double precision format of the computer programs has been retained for the present. Wherever necessary, asymptotic expansions similar to [B12] for case A4 were derived also for the other cases involving a finite system; they have been included in the computer solutions.

The numerical solution N1, listed in table 13, is based on a linear finite element approximation of the spatial derivatives in the transport equation and a third-order finite difference approximation of the time derivative. The theoretical basis of this particular scheme is discussed elsewhere (van Genuchten *1977* , van Genuchten and Gray *1978*) and will not be reviewed here. The program assumes that the nodal spacing (DELX) and the time increment (DELT) remain constant.

Table 2.--List of the most significant variables in the computer programs

Variable	Definition
APRX	Variable to indicate if the solution for a semi-infinite system can be used to approximate the solution for a finite system: APRX $= x/L - 0.9 + 8/P$. (A3, C8).
BETA	Dummy variable for the I-th eigenvalue, G(I). (A3, C8).
C	Dummy variable for concentration, c.
C(I)	Nodal values of concentration (N1).
CO	Constant input concentration, C_o.
CA, CB	Constants (C_a, C_b) in several boundary conditions (see table 1). (B14, N1).
CI	Constant initial concentration, C_i.
CONC	Concentration, c.
CONS(V,D,R,...)	Subroutine to calculate the concentration for a finite profile (A3, C8).
D	Dispersion coefficient.
DBND	Constant (α) in several boundary conditions (see table 1). (B14, C8).
DELT	Time increment in numerical solution (N1).
DELX	Nodal distance in numerical solution (N1).
DONE	First-order rate coefficient for decay, μ. (C8, N1).
DT	Increment in time for computer printout.
DX	Increment in distance for computer printout.
DZERO	Zero-order rate coefficient for production, γ. (B14, N1).

Table 2.--List of the most significant variables in the computer programs--Continued

Variable	Definition
EIGEN1(P)	Subroutine to calculate the first 20 eigen-values (β_i) for the series solution of a finite profile with a first-type boundary condition (A3).
EIGEN3(P)	Subroutine to calculate the first 20 eigen-values (β_i) for the series solution of a finite profile with a third-type boundary condition (C8).
EXF(A,B)	Function to calculate exp(A) erfc(B).
G(I)	Vector containing the first 20 eigen-values (β_i) for the series solutions (A3, C8).
KINIT	Input code for the initial condition in the numerical solution. If KINIT = -1, the constant initial concentration (CI) is read in: if KINIT = 0, the initial concentration is specified in the program itself; if KINIT = 1, the individual nodal values of the concentration, C(I), are read in separately (N1).
KSURF	Input code for the upper boundary condition in the numerical solution. If KSURF = 1, a first-type boundary condition is specified; if KSURF = 3, a third-type boundary condition is specified (N1).
N	Number of terms in the series solution; if N equals zero in the printout, the approximate solution was used (A3, C8).
NC	Number of examples considered in each program.
NE	Number of elements in the numerical solution (N1).
NN	Number of nodes in the numerical solution: NN = NE + 1 (N1).
NSTEPS	Number of time steps in the numerical solution (N1).

Table 2.--List of the most significant variables in the computer programs--Continued

Variable	Definition
P	Column Peclet number: P = vL/D.
R	Retardation factor.
T	Dummy variable for t or $(t-t_o)$.
TO	Duration of tracer pulse added to profile, t_o.
TI	Initial time for computer printout.
TIME	Time, t.
TITLE(I)	Vector containing information of title card (input label).
TM	Final time for computer printout.
TOL	Convergence criterion for series solution (A3, C8).
V	Average pore-water velocity, v.
VVO	Dimensionless time: VVO = vt/x. Equals number of pore volumes if x = L.
X	Distance, x.
X(I)	Nodal coordinates in numerical solution (N1).
XI	Initial distance for computer printout.
XL	Column length, L. (A3, C8).
XM	Maximum distance for computer printout.

Table 3.--Sample input data for the 5 computer programs listed in this bulletin

Program	Column: Card	1234567890 1	1234567890 2	1234567890 3	1234567890 4	1234567890 5	1234567890 6	1234567890 7	1234567890 8
A1	1	2							
	2	EXAMPLE A1-1	(P=5)						
	3	1.0	4.0	1.0	1000.0	.0	1.0		
	4	.0	2.0	20.0	5.0	5.0	25.0		
	5	EXAMPLE A1-2							
	6	25.0	37.5	3.0	5.0	.0	1.0		
	7	100.0	.0	100.0	1.0	1.0	30.0		
A3	1	2							
	2	EXAMPLE A3-1	(P=5)						
	3	1.0	4.0	1.0	1000.0	.0	1.0	.0001	
	4	.0	2.0	20.0	20.0	5.0	5.0	25.0	
	5	EXAMPLE A3-2							
	6	25.0	37.5	3.0	5.0	.0	1.0	.0001	
	7	100.0	.0	100.0	100.0	1.0	1.0	30.0	
B14	1	1							
	2	EXAMPLE B14-1							
	3	25.0	37.5	3.0	.5	.25	.0	.0	10.0
	4	.0	5.0	100.0	2.5	2.5	7.5		
C8	1	2							
	2	EXAMPLE C8-1	(P=5)						
	3	1.0	4.0	1.0	1000.0	.5	.25	.0	1.0
	4	.0	2.0	20.0	20.0	5.0	5.0	25.0	.0001
	5	EXAMPLE C8-2							
	6	25.0	37.5	3.0	5.0	5.0	.25	.0	1.0
	7	.0	5.0	100.0	100.0	2.5	2.5	12.5	.0001
N1	1	2							
	2	EXAMPLE A3-1	(P=5)						
	3	40 125	1 -1	.5	.2	5.0	.0	.0	.0
	4	1.0	4.0	1.0	.0	1.0	.0	1000.0	
	5	EXAMPLE B14-1							
	6	40 125	3 -1	2.5	.1	2.5	.5	.0	.25
	7	25.0	37.5	3.0	.0	.0	10.0	1000.0	

Table 4.--Fortran listing of the function EXF(A,B) = exp(A) erfc(B)

EXF

```
      FUNCTICN EXF(A,B)
C
C     PURPOSE: TO CALCULATE EXP(A) ERFC(B)
C
      IMPLICIT REAL*8 (A-H,O-Z)
      EXF=0.0
      IF((DABS(A).GT.170.).AND.(B.LE.0.)) RETURN
      IF(B.NE.0.0) GO TO 1
      EXF=DEXP(A)
      RETURN
    1 C=A-B*B
      IF((DABS(C).GT.170.).AND.(B.GT.0.)) RETURN
      IF(C.LT.-170.) GO TO 4
      X=DABS(B)
      IF(X.GT.3.0) GO TO 2
      T=1./(1.+.3275911*X)
      Y=T*(.2548296-T*(.2844967-T*(1.421414-T*(1.453152-1.061405*T))))
      GO TO 3
    2 Y=.5641896/(X+.5/(X+1./(X+1.5/(X+2./(X+2.5/(X+1.))))))
    3 EXF=Y*DEXP(C)
    4 IF(B.LT.0.0) EXF=2.*DEXP(A)-EXF
      RETURN
      END
```

Table 5.--Fortran listing of computer program A1. The function EXF is listed in table 4

MAIN

```
C
C
C     ******************************************************************
C     *                                                                *
C     *        ONE-DIMENSIONAL CCNVECTIVE-DISPERSIVE EQUATION      A1  *
C     *                                                                *
C     *        SEMI-INFINITE PRCFILE                                   *
C     *                                                                *
C     *        NO PRODUCTION OR CECAY                                  *
C     *        LINEAR ADSORPTICN (R)                                   *
C     *        CONSTANT INITIAL CONCENTRATION (CI)                     *
C     *        INPUT CONCENTRATICN   = CO (T.LE.TO)                    *
C     *                              = 0  (T.GT.TO)                    *
C     *                                                                *
C     ******************************************************************
C
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION TITLE(20)
C
C     ----- READ NUMBER OF CURVES TO BE CALCULATED -----
      READ(5,1000) NC
      DO 4 K=1,NC
      READ(5,1001) TITLE
      WRITE(6,1002) TITLE
C
C     ----- READ AND WRITE INPUT PARAMETERS -----
      READ(5,1003) V,D,R,TO,CI,CO
      READ(5,1003) XI,DX,XM,TI,DT,TM
      WRITE(6,1004) V,D,R,TO,CI,CO
C
C     ---------------
      D=D/R
      V=V/R
      IF(DX.EQ.0.) DX=1.0
      IF(DT.EQ.0.) DT=1.0
      IMAX=(XM+DX-XI)/DX
      JMAX=(TM+DT-TI)/DT
      E=0.0
      DO 4 J=1,JMAX
      IF(IMAX.GE.J) WRITE(6,1005)
      TIME=TI+(J-1)*DT
      DO 4 I=1,IMAX
      X=XI+(I-1)*DX
      VVO=0.0
      IF(X.EQ.0.) GO TO 1
      VVO=V*R*TIME/X
    1 DO 2 M=1,2
      A1=0.0
```

```
      A2=0.0
      T=TIME+(1-M)*TO
      IF(T.LE.0.) GO TO 2
      CM=(X-V*T)/DSQRT(4.*D*T)
      CP=(X+V*T)/DSQRT(4.*D*T)
      Q=V*X/D
      A1=0.5*(EXF(E,CM)+EXF(Q,CP))
      A2=0.5*EXF(E,CM)+V*DSQRT(.3183099*T/D)*EXF(-CM*CM,E)-0.5*(1.+Q+V*V
     1*T/D)*EXF(Q,CP)
      IF(M.EQ.2) GO TO 3
      CONC1=CI+(CO-CI)*A1
      CONC2=CI+(CO-CI)*A2
    2 CONTINUE
    3 CONC1=CONC1-CO*A1
      CONC2=CONC2-CO*A2
    4 WRITE(6,1006) X,TIME,VVC,CCNC1,CONC2
C
C     ---------------
 1000 FORMAT(I5)
 1001 FCRMAT(20A4)
 1002 FORMAT(1H1,10X,82(1H*)/11X,1H*,80X,1H*/11X,1H*,9X,'ONE-DIMENSIONAL
     1 CONVECTIVE-DISPERSIVE EQUATION',25X,1H*/11X,1H*,80X,1H*/11X,1H*,
     29X,'SEMI-INFINITE PROFILE',50X,1H*/11X,1H*,9X,'NO PRODUCTION AND D
     3ECAY',48X,1H*/11X,1H*,9X,'LINEAR ADSORPTION (R)',50X,1H*/11X,1H*,9
     4X,'CONSTANT INITIAL CCNCENTRATION (CI)',36X,1H*/11X,1H*,9X,'INPUT
     5CONCENTRATION = CO (T.LE.TO)',37X,1H*/11X,1H*,29X,'=  0 (T.GT.TO)'
     6,37X,1H*/11X,1H*,80X,1H*/11X,1H*,20A4,1H*/11X,1H*,80X,1H*/11X,82(1
     7H*))
 1003 FORMAT(8F10.0)
 1004 FORMAT(//11X,'INPUT PARAMETERS'/11X,16(1H=)//11X,'V =',F12.4,15X,'
     1D =',F12.4/11X,'R =',F12.4,15X,'TO =',F11.4/11X,'CI =',F11.4,15X,'
     2CO =',F11.4)
 1005 FORMAT(///11X,'DISTANCE',11X,'TIME',7X,'PORE VOLUME',12X,'CONCENTR
     1ATION'/14X,'(X)',13X,'(T)',11X,'(VVO)',6X,'FIRST-TYPE BC',4X,'THIR
     2D-TYPE BC')
 1006 FORMAT(4X,3(5X,F10.4),3X,F12.4,5X,F12.4)
      STOP
      END
```

Table 6.--Sample output from computer program A1

```
*****************************************************************************
*                                                                           *
*         ONE-DIMENSIONAL CONVECTIVE-DISPERSIVE EQUATION                    *
*                                                                           *
*         SEMI-INFINITE PROFILE                                             *
*         NO PRODUCTION AND DECAY                                           *
*         LINEAR ADSORPTION (R)                                             *
*         CONSTANT INITIAL CONCENTRATION (CI)                               *
*         INPUT CONCENTRATION = CO (T.LE.TO)                                *
*                             =  0 (T.GT.TO)                                *
*                                                                           *
*         EXAMPLE A1-1   (P=5)                                              *
*                                                                           *
*****************************************************************************
```

INPUT PARAMETERS
================

V =	1.0000	D =	4.0000
R =	1.0000	TO =	1000.0000
CI =	0.0	CO =	1.0000

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION FIRST-TYPE BC	CONCENTRATION THIRD-TYPE BC
0.0	5.0000	0.0	1.0000	0.7640
2.0000	5.0000	2.5000	0.9036	0.6376
4.0000	5.0000	1.2500	0.7731	0.5023
6.0000	5.0000	0.8333	0.6209	0.3712
8.0000	5.0000	0.6250	0.4648	0.2559
10.0000	5.0000	0.5000	0.3224	0.1638
12.0000	5.0000	0.4167	0.2064	0.0970
14.0000	5.0000	0.3571	0.1215	0.0530
16.0000	5.0000	0.3125	0.0655	0.0266
18.0000	5.0000	0.2778	0.0324	0.0123
20.0000	5.0000	0.2500	0.0146	0.0052

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION FIRST-TYPE BC	CONCENTRATION THIRD-TYPE BC
0.0	10.0000	0.0	1.0000	0.8845
2.0000	10.0000	5.0000	0.9626	0.8198
4.0000	10.0000	2.5000	0.9086	0.7424
6.0000	10.0000	1.6667	0.8377	0.6548
8.0000	10.0000	1.2500	0.7517	0.5610
10.0000	10.0000	1.0000	0.6544	0.4657
12.0000	10.0000	0.8333	0.5512	0.3738
14.0000	10.0000	0.7143	0.4481	0.2895
16.0000	10.0000	0.6250	0.3508	0.2161
18.0000	10.0000	0.5556	0.2641	0.1551
20.0000	10.0000	0.5000	0.1909	0.1070

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION FIRST-TYPE BC	CONCENTRATION THIRD-TYPE BC
0.0	15.0000	0.0	1.0000	0.9365
2.0000	15.0000	7.5000	0.9818	0.9003

4.0000	15.0000	3.7500	0.9549	0.8549
6.0000	15.0000	2.5000	0.9181	0.8004
8.0000	15.0000	1.8750	0.8707	0.7375
10.0000	15.0000	1.5000	0.8129	0.6677
12.0000	15.0000	1.2500	0.7456	0.5931
14.0000	15.0000	1.0714	0.6707	0.5161
16.0000	15.0000	0.9375	0.5907	0.4394
18.0000	15.0000	0.8333	0.5087	0.3656
20.0000	15.0000	0.7500	0.4278	0.2969

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION FIRST-TYPE BC	CONCENTRATION THIRD-TYPE BC
0.0	20.0000	0.0	1.0000	0.9630
2.0000	20.0000	10.0000	0.9902	0.9416
4.0000	20.0000	5.0000	0.9756	0.9142
6.0000	20.0000	3.3333	0.9551	0.8801
8.0000	20.0000	2.5000	0.9278	0.8392
10.0000	20.0000	2.0000	0.8933	0.7916
12.0000	20.0000	1.6667	0.8511	0.7379
14.0000	20.0000	1.4286	0.8014	0.6788
16.0000	20.0000	1.2500	0.7449	0.6157
18.0000	20.0000	1.1111	0.6827	0.5501
20.0000	20.0000	1.0000	0.6162	0.4837

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION FIRST-TYPE BC	CONCENTRATION THIRD-TYPE BC
0.0	25.0000	0.0	1.0000	0.9776
2.0000	25.0000	12.5000	0.9944	0.9646
4.0000	25.0000	6.2500	0.9860	0.9476
6.0000	25.0000	4.1667	0.9740	0.9261
8.0000	25.0000	3.1250	0.9578	0.8995
10.0000	25.0000	2.5000	0.9368	0.8677
12.0000	25.0000	2.0833	0.9103	0.8304
14.0000	25.0000	1.7857	0.8780	0.7879
16.0000	25.0000	1.5625	0.8399	0.7404
18.0000	25.0000	1.3889	0.7960	0.6886
20.0000	25.0000	1.2500	0.7467	0.6334

```
*****************************************************************************
*                                                                           *
*         ONE-DIMENSIONAL CONVECTIVE-DISPERSIVE EQUATION                    *
*                                                                           *
*         SEMI-INFINITE PROFILE                                             *
*         NO PRODUCTION AND DECAY                                           *
*         LINEAR ADSORPTION (R)                                             *
*         CONSTANT INITIAL CONCENTRATION (CI)                               *
*         INPUT CONCENTRATION = CO (T.LE.TO)                                *
*                             =  0 (T.GT.TO)                                *
*                                                                           *
*         EXAMPLE A1-2                                                      *
*                                                                           *
*****************************************************************************
```

INPUT PARAMETERS
================

```
V  =     25.0000              D  =     37.5000
R  =      3.0000              TO =      5.0000
CI =      0.0                 CO =      1.0000
```

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION FIRST-TYPE BC	CONCENTRATION THIRD-TYPE BC
100.0000	1.0000	0.2500	0.0000	0.0000
100.0000	2.0000	0.5000	0.0000	0.0000
100.0000	3.0000	0.7500	0.0000	0.0000
100.0000	4.0000	1.0000	0.0000	0.0000
100.0000	5.0000	1.2500	0.0000	0.0000
100.0000	6.0000	1.5000	0.0000	0.0000
100.0000	7.0000	1.7500	0.0010	0.0008
100.0000	8.0000	2.0000	0.0113	0.0088
100.0000	9.0000	2.2500	0.0563	0.0465
100.0000	10.0000	2.5000	0.1655	0.1439
100.0000	11.0000	2.7500	0.3378	0.3059
100.0000	12.0000	3.0000	0.5332	0.4987
100.0000	13.0000	3.2500	0.6975	0.6700
100.0000	14.0000	3.5000	0.7802	0.7684
100.0000	15.0000	3.7500	0.7509	0.7592
100.0000	16.0000	4.0000	0.6228	0.6474
100.0000	17.0000	4.2500	0.4485	0.4795
100.0000	18.0000	4.5000	0.2840	0.3124
100.0000	19.0000	4.7500	0.1607	0.1816
100.0000	20.0000	5.0000	0.0825	0.0956
100.0000	21.0000	5.2500	0.0389	0.0462
100.0000	22.0000	5.5000	0.0171	0.0208
100.0000	23.0000	5.7500	0.0071	0.0088
100.0000	24.0000	6.0000	0.0028	0.0035
100.0000	25.0000	6.2500	0.0010	0.0013
100.0000	26.0000	6.5000	0.0004	0.0005
100.0000	27.0000	6.7500	0.0001	0.0002
100.0000	28.0000	7.0000	0.0000	0.0001
100.0000	29.0000	7.2500	0.0000	0.0000
100.0000	30.0000	7.5000	0.0000	0.0000

Table 7.--Fortran listing of computer program A3. The function EXF is listed in table 4

MAIN

```
C
C
C
C     ******************************************************************
C     *                                                                *
C     *       ONE-DIMENSICNAL CCNVECTIVE DISPERSIVE EQUATION      A3   *
C     *                                                                *
C     *       FIRST-TYPE BOUNDARY CONDITION                            *
C     *       FINITE PROFILE                                           *
C     *                                                                *
C     *       NO PRODUCTICN CR DECAY                                   *
C     *       LINEAR ADSORPTICN (R)                                    *
C     *       CONSTANT INITIAL CCNCENTRATION (CI)                      *
C     *       INPUT CONCENTRATION    = CO (T.LE.TO)                    *
C     *                              =  0 (T.GT.TO)                    *
C     *                                                                *
C     ******************************************************************
C
C
      IMPLICIT REAL*8 (A-H,C-Z)
      CCMMCN G(20)
      DIMENSICN TITLE(20)
C
C     ----- READ NUMBER OF CURVES TO BE GENERATED -----
      READ(5,1000) NC
      DO 4 K=1,NC
      READ(5,1001) TITLE
      WRITE(6,1002) TITLE
C     ----- READ AND WRITE INPUT PARAMETERS -----
      READ(5,1003) V,D,R,TO,CI,CO,TOL
      READ(5,1003) XI,DX,XM,XL,TI,DT,TM
      WRITE(6,1004) V,D,R,TO,CI,CO,XL,TOL
C
C     ---------------
      D=D/R
      V=V/R
      IF(DX.EQ.0.) DX=1.0
      IF(DT.EQ.0.) DT=1.0
      XM=DMIN1(XM,XL)
      P=V*XL/D
      IMAX=(XM+DX-XI)/DX
      JMAX=(TM+DT-TI)/DT
      IF(P.LE.100.) CALL EIGEN1(P)
      DO 4 J=1,JMAX
      TIME=TI+(J-1)*DT
      IF(IMAX.GE.J) WRITE(6,1005)
      DO 4 I=1,IMAX
      X=XI+(I-1)*DX
```

```
      VVO=0.0
      IF(X.EQ.0.) GO TO 1
      VVO=V*R*TIME/X
    1 DO 2 M=1,2
      C=0.0
      T=TIME+(1-M)*TO
      IF(T.LE.0.) GO TO 2
      CALL CCNS(C,V,D,X,T,XL,TOL,N)
      IF(M.EQ.2) GO TO 3
      CCNC=CI+(CO-CI)*C
    2 CONTINUE
    3 CCNC=CCNC-CO*C
    4 WRITE(6,1006) X,TIME,VVC,CCNC,N
C
C     ----------------
 1000 FORMAT(I5)
 1001 FORMAT(20A4)
 1002 FORMAT(1H1,10X,82(1H*)/11X,1H*,80X,1H*/11X,1H*,9X,'ONE-DIMENSIONAL
     1 CONVECTIVE-DISPERSIVE EQUATION',25X,1H*/11X,1H*,80X,1H*/11X,1H*,9
     2X,'FIRST-TYPE BOUNDARY CONDITION',42X,1H*/11X,1H*,9X,'FINITE PROFI
     3LE',57X,1H*/11X,1H*,80X,1H*/11X,1H*,9X,'NO PRODUCTION OR DECAY',49
     4X,1H*/11X,1H*,9X,'LINEAR ADSORPTION (R)',50X,1H*/11X,1H*,9X,'CONST
     5ANT INITIAL CONCENTRATICN (CI)',36X,1H*/11X,1H*,9X,'INPUT CONCENTR
     6ATION = CO (T.LE.TO)',37X,1H*/11X,1H*,29X,'=  0 (T.GT.TO)',37X,1H*
     7/11X,1H*,80X,1H*/11X,1H*,20A4,1H*/11X,1H*,80X,1H*/11X,82(1H*))
 1003 FORMAT(8F10.0)
 1004 FORMAT(//11X,'INPUT PARAMETERS'/11X,16(1H=)//11X,'V =',F12.4,15X,'
     1D =',F12.4/11X,'R =',F12.4,15X,'TO =',F11.4/11X,'CI =',F11.4,15X,'
     2CO =',F11.4/11X,'XL =',F11.4,15X,'TOL =',F10.6)
 1005 FORMAT(///11X,'DISTANCE',11X,'TIME',7X,'PORE VOLUME',6X,'CONCENTRA
     1TION',3X,'NUMBER'/14X,'(X)',13X,'(T)',11X,'(VVO)',14X,'(C)',7X,'OF
     2 TERMS')
 1006 FORMAT(4X,3(5X,F10.4),8X,F10.4,7X,I4)
      STOP
      END
```

EIGEN1

```
      SUBROUTINE EIGEN1(P)
C
C     PURPOSE: TO CALCULATE THE EIGENVALUES
C
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON G(20)
      BETA=0.1
      DO 4 I=1,20
      J=0
    1 J=J+1
      IF(J.GT.15) GO TO 3
      DELTA=-0.2*(-0.5)**J
    2 BET2=BETA
      BETA=BETA+DELTA
      A=BET2*DCOS(BET2)+0.5*P*DSIN(BET2)
      B=BETA*DCOS(BETA)+0.5*P*DSIN(BETA)
      IF(A*B) 1,3,2
    3 G(I)=(BET2*B-BETA*A)/(B-A)
    4 BETA=BETA+0.2
      WRITE(6,1000) (G(I),I=1,20)
 1000 FORMAT(//11X,'CALCULATED EIGENVALUES'/11X,22(1H=)/(8X,5F12.6/))
      RETURN
      END
```

CCNS

```
      SUBROUTINE CONS(C,V,D,X,T,XL,TOL,I)
C
C     PURPOSE: TO CALCULATE CONCENTRATION C
C
      IMPLICIT REAL*8 (A-H,C-Z)
      COMMCN G(20)
      I=0
      P=V*XL/D
      Q=V*X/D
      APRX=X/XL-0.9+8./P
      IF(APRX.LT.0.) GO TO 4
      IF((P.GT.100.).OR.((P-40.*V*T/XL).GT.5.)) GO TO 4
      EX=0.5*Q-0.25*V*V*T/D
C
C     -----SERIES SOLUTION-----
      SUM=0.0
      IF(X.EQ.0.) GO TO 3
      DO 2 J=1,10
      DSUM=0.0
      DO 1 K=1,2
      I=2*J+K-2
      A=G(I)*DSIN(G(I)*X/XL)
      IF(DABS(A).LT.1.D-10) A=0.0
      EXP=EX-(G(I)/XL)**2*D*T
      IF(DABS(EXP).GT.160.) EXP=-160.
    1 DSUM=DSUM+DEXP(EXP)*A/(G(I)**2+0.25*P*P+0.5*P)
      SUM=SUM+DSUM
      IF(DABS(DSUM/SUM).LT.TCL) GO TO 3
    2 CONTINUE
      GO TO 4
    3 C=1.-2.*SUM
      RETURN
C
C     ----- APPROXIMATE SOLLTICN -----
    4 S=DSQRT(4.*D*T)
      E=0.0
      C=0.5*(EXF(E,(X-V*T)/S)+EXF(Q,(X+V*T)/S))
      IF(APRX.LT.0.) RETURN
      A=2.*D*T/(2.*XL-X+V*T)**2
      B=2.*V*T/(2.*XL-X)
      C=C+(2.*XL-X)*A*EXF(P-0.5/A,E)*(1.-A*((1.-B)-3.*A*((1.-2.*B)-5.*A*
     1((1.-3.*B)-7.*A*(1.-4.*B)))))/DSQRT(3.141593*D*T)
      RETURN
      END
```

Table 8.--Sample output from computer program A3

```
*******************************************************************************
*                                                                             *
*        ONE-DIMENSIONAL CONVECTIVE-DISPERSIVE EQUATION                       *
*                                                                             *
*        FIRST-TYPE BOUNDARY CONDITION                                        *
*        FINITE PROFILE                                                       *
*                                                                             *
*        NO PRODUCTION OR DECAY                                               *
*        LINEAR ADSORPTION (R)                                                *
*        CONSTANT INITIAL CONCENTRATION (CI)                                  *
*        INPUT CONCENTRATION = CO (T.LE.TO)                                   *
*                            =  0 (T.GT.TO)                                   *
*                                                                             *
*        EXAMPLE A3-1   (P=5)                                                 *
*                                                                             *
*******************************************************************************
```

INPUT PARAMETERS
================

V =	1.0000	D =	4.0000
R =	1.0000	TO =	1000.0000
CI =	0.0	CO =	1.0000
XL =	20.0000	TOL =	0.000100

CALCULATED EIGENVALUES
======================

2.380644	5.163306	8.151564	11.214906	14.310123
17.421289	20.541462	23.667186	26.796564	29.928469
33.062194	36.197272	39.333382	42.470298	45.607854
48.745928	51.884426	55.023276	58.162421	61.301816

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION (C)	NUMBER OF TERMS
0.0	5.0000	0.0	1.0000	0
2.0000	5.0000	2.5000	0.9036	6
4.0000	5.0000	1.2500	0.7731	6
6.0000	5.0000	0.8333	0.6209	6
8.0000	5.0000	0.6250	0.4648	6
10.0000	5.0000	0.5000	0.3225	6
12.0000	5.0000	0.4167	0.2064	6
14.0000	5.0000	0.3571	0.1216	6
16.0000	5.0000	0.3125	0.0661	6
18.0000	5.0000	0.2778	0.0348	6
20.0000	5.0000	0.2500	0.0240	6

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION (C)	NUMBER OF TERMS
0.0	10.0000	0.0	1.0000	0
2.0000	10.0000	5.0000	0.9626	6
4.0000	10.0000	2.5000	0.9086	6

6.0000	10.0000	1.6667	0.8378	6
8.0000	10.0000	1.2500	0.7520	6
10.0000	10.0000	1.0000	0.6553	6
12.0000	10.0000	0.8333	0.5536	6
14.0000	10.0000	0.7143	0.4544	6
16.0000	10.0000	0.6250	0.3666	6
18.0000	10.0000	0.5556	0.3013	6
20.0000	10.0000	0.5000	0.2747	6

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION (C)	NUMBER OF TERMS
0.0	15.0000	0.0	1.0000	0
2.0000	15.0000	7.5000	0.9819	6
4.0000	15.0000	3.7500	0.9553	6
6.0000	15.0000	2.5000	0.9189	4
8.0000	15.0000	1.8750	0.8726	4
10.0000	15.0000	1.5000	0.8170	4
12.0000	15.0000	1.2500	0.7544	4
14.0000	15.0000	1.0714	0.6889	4
16.0000	15.0000	0.9375	0.6271	4
18.0000	15.0000	0.8333	0.5788	4
20.0000	15.0000	0.7500	0.5586	6

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION (C)	NUMBER OF TERMS
0.0	20.0000	0.0	1.0000	0
2.0000	20.0000	10.0000	0.9905	4
4.0000	20.0000	5.0000	0.9764	4
6.0000	20.0000	3.3333	0.9569	4
8.0000	20.0000	2.5000	0.9316	4
10.0000	20.0000	2.0000	0.9005	4
12.0000	20.0000	1.6667	0.8648	4
14.0000	20.0000	1.4286	0.8266	4
16.0000	20.0000	1.2500	0.7899	4
18.0000	20.0000	1.1111	0.7608	4
20.0000	20.0000	1.0000	0.7485	4

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION (C)	NUMBER OF TERMS
0.0	25.0000	0.0	1.0000	0
2.0000	25.0000	12.5000	0.9949	4
4.0000	25.0000	6.2500	0.9872	4
6.0000	25.0000	4.1667	0.9766	4
8.0000	25.0000	3.1250	0.9626	4
10.0000	25.0000	2.5000	0.9455	4
12.0000	25.0000	2.0833	0.9255	4
14.0000	25.0000	1.7857	0.9041	4
16.0000	25.0000	1.5625	0.8833	4
18.0000	25.0000	1.3889	0.8668	4
20.0000	25.0000	1.2500	0.8598	4

```
*******************************************************************************
*                                                                             *
*         ONE-DIMENSIONAL CONVECTIVE-DISPERSIVE EQUATION                      *
*                                                                             *
*         FIRST-TYPE BOUNDARY CONDITION                                       *
*         FINITE PROFILE                                                      *
*                                                                             *
*         NO PRODUCTION OR DECAY                                              *
*         LINEAR ADSORPTION (R)                                               *
*         CONSTANT INITIAL CONCENTRATION (CI)                                 *
*         INPUT CONCENTRATION = CO (T.LE.TO)                                  *
*                             =  0 (T.GT.TO)                                  *
*                                                                             *
*         EXAMPLE A3-2                                                        *
*                                                                             *
*******************************************************************************
```

INPUT PARAMETERS
================

V =	25.0000	D =	37.5000
R =	3.0000	TO =	5.0000
CI =	0.0	CO =	1.0000
XL =	100.0000	TOL =	0.000100

CALCULATED EIGENVALUES
======================

3.050337	6.102126	9.156690	12.215114	15.278191
18.346412	21.419993	24.498930	27.583053	30.672083
33.765678	36.863467	39.965076	43.070143	46.178327
49.289314	52.402819	55.518585	58.636381	61.756003

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION (C)	NUMBER OF TERMS
100.0000	1.0000	0.2500	0.0000	0
100.0000	2.0000	0.5000	0.0000	0
100.0000	3.0000	0.7500	0.0000	0
100.0000	4.0000	1.0000	0.0000	0
100.0000	5.0000	1.2500	0.0000	0
100.0000	6.0000	1.5000	0.0000	0
100.0000	7.0000	1.7500	0.0013	0
100.0000	8.0000	2.0000	0.0138	0
100.0000	9.0000	2.2500	0.0660	0
100.0000	10.0000	2.5000	0.1872	0
100.0000	11.0000	2.7500	0.3697	0
100.0000	12.0000	3.0000	0.5677	0
100.0000	13.0000	3.2500	0.7250	0
100.0000	14.0000	3.5000	0.7920	0
100.0000	15.0000	3.7500	0.7427	0
100.0000	16.0000	4.0000	0.5983	0
100.0000	17.0000	4.2500	0.4174	0
100.0000	18.0000	4.5000	0.2557	0
100.0000	19.0000	4.7500	0.1399	0

100.0000	20.0000	5.0000	0.0694	0
100.0000	21.0000	5.2500	0.0317	0
100.0000	22.0000	5.5000	0.0135	0
100.0000	23.0000	5.7500	0.0054	0
100.0000	24.0000	6.0000	0.0020	12
100.0000	25.0000	6.2500	0.0007	10
100.0000	26.0000	6.5000	0.0003	10
100.0000	27.0000	6.7500	0.0001	10
100.0000	28.0000	7.0000	0.0000	10
100.0000	29.0000	7.2500	0.0000	10
100.0000	30.0000	7.5000	0.0000	10

Table 9.--Fortran listing of computer program B14. The function EXF is listed in table 4

MAIN

```
C
C
C     ***************************************************************
C     *                                                             *
C     *       ONE-DIMENSIONAL CONVECTIVE-DISPERSIVE EQUATION    B14 *
C     *                                                             *
C     *       THIRD-TYPE BOUNDARY CONDITION                         *
C     *       SEMI-INFINITE PROFILE                                 *
C     *                                                             *
C     *       ZERO-ORDER PRODUCTION (DZERO)                         *
C     *       LINEAR ADSORPTION (R)                                 *
C     *       CONSTANT INITIAL CONCENTRATION (CI)                   *
C     *       INPUT CONCENTRATION = CA+CB*EXP(-DBND*T)              *
C     *                                                             *
C     ***************************************************************
C
      IMPLICIT REAL*8 (A-H,C-Z)
      DIMENSION TITLE(20)
C
C     ----- READ NUMBER OF CURVES TO BE CALCULATED -----
      READ(5,1000) NC
      DO 4 K=1,NC
      READ(5,1001) TITLE
      WRITE(6,1002) TITLE
C
C     ----- READ AND WRITE INPUT PARAMETERS -----
      READ(5,1003) V,D,R,DZERO,DBND,CI,CA,CB
      READ(5,1003) XI,DX,XM,TI,DT,TM
      WRITE(6,1004) V,D,R,DZERO,DBND,CI,CA,CB
C
C     ---------------
      D=D/R
      V=V/R
      DZERO=DZERO/R
      S=V**2-4.*DBND*D
      IF(S.LE.0.) GO TO 5
      Y=DSQRT(S)
      IF(DX.EQ.0.) DX=1.0
      IF(DT.EQ.0.) DT=1.0
      IMAX=(XM+DX-XI)/DX
      JMAX=(TM+DT-TI)/DT
      DO 4 J=1,JMAX
      T=TI+(J-1)*DT
      IF(IMAX.GE.J) WRITE(6,1005)
      DO 4 I=1,IMAX
      X=XI+(I-1)*DX
      VVO=0.0
      IF(X.EQ.0.) GO TO 1
```

```
      VVO=V*R*T/X
    1 P=V*X/D
      S=DSQRT(4.*D*T)
      A1=X-V*T
      A2=X+V*T
      AM=0.5*EXF(0.D0,A1/S)
      AP=0.5*EXF(P,A2/S)
      AZ=DSQRT(.3183099*T/D)*EXF(-(A1/S)**2,0.D0)
      BM=(X-Y*T)/S
      BP=(X+Y*T)/S
      CM=0.5*(V-Y)*X/D
      CP=0.5*(V+Y)*X/D
      A=AM+V*AZ-(1.+P+V*V*T/D)*AP
      B=DEXP(-DBND*T)*(V/(V+Y)*EXF(CM,BM)+V/(V-Y)*EXF(CP,BP))-V*V*AP/(DB
     1ND*D)
      CONC=CI+(CA-CI)*A+CB*B+DZERO*(T+(A1+D/V)*AM/V-.5*(A2+2.*D/V)*AZ+(T
     1-D/V**2+.5*A2**2/D)*AP)
    4 WRITE(6,1006) X,T,VVO,CONC
      GO TO 6
    5 WRITE(6,1007)
    6 CONTINUE
C
C     ---------------
 1000 FORMAT(I5)
 1001 FORMAT(20A4)
 1002 FORMAT(1H1,10X,82(1H*)/11X,1H*,80X,1H*/11X,1H*,9X,'ONE-DIMENSIONAL
     1 CONVECTIVE-DISPERSIVE EQUATION',25X,1H*/11X,1H*,80X,1H*,/11X,1H*,
     29X,'THIRD-TYPE BOUNDARY CONDITION',42X,1H*/11X,1H*,9X,'SEMI-INFINI
     3TE PROFILE',50X,1H*/11X,1H*,80X,1H*/11X,1H*,9X,'LINEAR ADSORPTION
     4(R)',50X,1H*/11X,1H*,9X,'ZERO-ORDER PRODUCTION (DZERO)',42X,1H*/11
     5X,1H*,9X,'CONSTANT INITIAL CONCENTRATION (CI)',36X,1H*/11X,1H*,9X,
     6'INPUT CONCENTRATION = CA+CB*EXP(-DBND*T)',31X,1H*/11X,1H*,80X,1H*
     7/11X,1H*,20A4,1H*/11X,1H*,80X,1H*/11X,82(1H*))
 1003 FORMAT(8F10.0)
 1004 FORMAT(//11X,'INPUT PARAMETERS'/11X,16(1H=)//11X,'V =',F12.4,15X,'
     1D =',F12.4/11X,'R =',F12.4,15X,'DZERO =',F8.4/11X,'DBND =',F9.4,15
     2X,'CI =',F11.4/11X,'CA =',F11.4,15X,'CB =',F11.4)
 1005 FORMAT(////11X,'DISTANCE',11X,'TIME',7X,'PORE VOLUME',6X,'CONCENTR
     1ATION'/14X,'(X)',13X,'(T)',11X,'(VVO)',14X,'(C)'/)
 1006 FORMAT(4X,3(5X,F10.4),8X,F10.4)
 1007 FORMAT(///5X/6(1H*),' DBND IS TOO LARGE, THIS CASE NOT EXECUTED ',
     16(1H*))
      STOP
      END
```

Table 10.--Sample output from computer program B14

```
*********************************************************************************
*                                                                               *
*        ONE-DIMENSIONAL CONVECTIVE-DISPERSIVE EQUATION                         *
*                                                                               *
*        THIRD-TYPE BOUNDARY CONDITION                                          *
*        SEMI-INFINITE PROFILE                                                  *
*                                                                               *
*        LINEAR ADSORPTION (R)                                                  *
*        ZERO-ORDER PRODUCTION (DZERO)                                          *
*        CONSTANT INITIAL CONCENTRATION (CI)                                    *
*        INPUT CONCENTRATION = CA+CB*EXP(-DBND*T)                               *
*                                                                               *
*        EXAMPLE B14-1                                                          *
*                                                                               *
*********************************************************************************
```

INPUT PARAMETERS
```
===============

V =       25.0000              D =       37.5000
R =        3.0000              DZERO =    0.5000
DBND =     0.2500              CI =       0.0
CA =       0.0                 CB =      10.0000
```

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION (C)
0.0	2.5000	0.0	5.6301
5.0000	2.5000	12.5000	6.5099
10.0000	2.5000	6.2500	6.9976
15.0000	2.5000	4.1667	6.5451
20.0000	2.5000	3.1250	4.9945
25.0000	2.5000	2.5000	3.0083
30.0000	2.5000	2.0833	1.4860
35.0000	2.5000	1.7857	0.7302
40.0000	2.5000	1.5625	0.4809
45.0000	2.5000	1.3889	0.4258
50.0000	2.5000	1.2500	0.4176
55.0000	2.5000	1.1364	0.4167
60.0000	2.5000	1.0417	0.4167
65.0000	2.5000	0.9615	0.4167
70.0000	2.5000	0.8929	0.4167
75.0000	2.5000	0.8333	0.4167
80.0000	2.5000	0.7812	0.4167
85.0000	2.5000	0.7353	0.4167
90.0000	2.5000	0.6944	0.4167
95.0000	2.5000	0.6579	0.4167
100.0000	2.5000	0.6250	0.4167

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION (C)
0.0	5.0000	0.0	3.0368
5.0000	5.0000	25.0000	3.6467

10.0000	5.0000	12.5000	4.3309
15.0000	5.0000	8.3333	5.0686
20.0000	5.0000	6.2500	5.7862
25.0000	5.0000	5.0000	6.3312
30.0000	5.0000	4.1667	6.4937
35.0000	5.0000	3.5714	6.1066
40.0000	5.0000	3.1250	5.1799
45.0000	5.0000	2.7778	3.9454
50.0000	5.0000	2.5000	2.7417
55.0000	5.0000	2.2727	1.8251
60.0000	5.0000	2.0833	1.2668
65.0000	5.0000	1.9231	0.9917
70.0000	5.0000	1.7857	0.8815
75.0000	5.0000	1.6667	0.8455
80.0000	5.0000	1.5625	0.8359
85.0000	5.0000	1.4706	0.8338
90.0000	5.0000	1.3889	0.8334
95.0000	5.0000	1.3158	0.8333
100.0000	5.0000	1.2500	0.8333

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION (C)
0.0	7.5000	0.0	1.8396
5.0000	7.5000	37.5000	2.0140
10.0000	7.5000	18.7500	2.4348
15.0000	7.5000	12.5000	2.9091
20.0000	7.5000	9.3750	3.4425
25.0000	7.5000	7.5000	4.0349
30.0000	7.5000	6.2500	4.6721
35.0000	7.5000	5.3571	5.3136
40.0000	7.5000	4.6875	5.8618
45.0000	7.5000	4.1667	6.2657
50.0000	7.5000	3.7500	6.3464
55.0000	7.5000	3.4091	6.0565
60.0000	7.5000	3.1250	5.4071
65.0000	7.5000	2.8846	4.5184
70.0000	7.5000	2.6786	3.5685
75.0000	7.5000	2.5000	2.7251
80.0000	7.5000	2.3438	2.0879
85.0000	7.5000	2.2059	1.6733
90.0000	7.5000	2.0833	1.4397
95.0000	7.5000	1.9737	1.3253
100.0000	7.5000	1.8750	1.2764

Table 11.--Fortran listing of computer program C8. The function EXF is listed in table 4

MAIN

```
C
C      ***********************************************************************
C      *                                                                     *
C      *       ONE-DIMENSICNAL CCNVECTIVE DISPERSIVE EQUATION       C8       *
C      *                                                                     *
C      *       FIRST-TYPE BOUNDARY CONDITION                                 *
C      *       FINITE PROFILE                                                *
C      *                                                                     *
C      *       ZERO-ORDER PRODUCTION (DZERO)                                 *
C      *       FIRST-ORDER DECAY (DONE)                                      *
C      *       LINEAR ADSORPTICN (R)                                         *
C      *       CONSTANT INITIAL CONCENTRATION (CI)                           *
C      *       INPUT CONCENTRATICN    = CO (T.LE.TO)                         *
C      *                              =  0 (T.GT.TO)                         *
C      *                                                                     *
C      ***********************************************************************
C
C
       IMPLICIT REAL*8 (A-H,C-Z)
       COMMON G(20)
       DIMENSION TITLE(20)
C
C      ----- READ NUMBER OF CURVES TO BE GENERATED -----
       READ(5,1000) NC
       DO 4 K=1,NC
       READ(5,1001) TITLE
       WRITE(6,1002) TITLE
C
C      ----- READ AND WRITE INPUT PARAMETERS -----
       READ(5,1003) V,D,R,TO,DZERO,DONE,CI,CO
       READ(5,1003) XI,DX,XM,XL,TI,DT,TM,TOL
       WRITE(6,1004) V,D,R,TC,DZERO,CI,DONE,CO,TOL
C
C      ---------------
       D=D/R
       V=V/R
       DZERO=DZERO/R
       DONE=DCNE/R
       DZD=DZERO/DONE
       IF(DX.EQ.0.) DX=1.0
       IF(DT.EQ.0.) DT=1.0
       XM=DMIN1(XM,XL)
       P=V*XL/D
       IMAX=(XM+DX-XI)/DX
       JMAX=(TM+DT-TI)/DT
       IF(P.LE.100.) CALL EIGEN3(P)
       DO 4 J=1,JMAX
       TIME=TI+(J-1)*DT
```

```
      IF(IMAX.GE.J) WRITE(6,1005)
      DO 4 I=1,IMAX
      X=XI+(I-1)*DX
      VVO=0.0
      IF(X.EQ.0.) GO TO 1
      VVO=V*R*TIME/X
    1 CALL CCNS(A,V,D,DONE,X,TIME,XL,TOL,N,0)
      CALL CCNS(B,V,D,DONE,X,TIME,XL,TOL,N,1)
      CONC=DZD+(CI-DZD)*A+(CO-DZD)*B
      T=TIME-TO
      IF(T.LE.0.) GO TO 2
      CALL CCNS(B,V,D,DONE,X,T,XL,TOL,N,1)
      CONC=CONC-CO*B
    2 CONTINUE
    4 WRITE(6,1006) X,TIME,VVO,CONC,N
C
C     ----------------
 1000 FORMAT(I5)
 1001 FORMAT(20A4)
 1002 FORMAT(1H1,10X,82(1H*)/11X,1H*,80X,1H*/11X,1H*,9X,'ONE-DIMENSIONAL
     1 CONVECTIVE-DISPERSIVE EQUATION',25X,1H*/11X,1H*,80X,1H*/11X,1H*,9
     2X,'THIRD-TYPE BOUNDARY CONDITION',42X,1H*/11X,1H*,9X,'FINITE PROFI
     3LE',57X,1H*/11X,1H*,80X,1H*/11X,1H*,9X,'ZERO-ORDER PRODUCTION (DZE
     4RO)',42X,1H*/11X,1H*,9X,'FIRST-ORDER DECAY (DONE)',47X,1H*/11X,1H*
     5,9X,'LINEAR ADSORPTION (R)',50X,1H*/11X,1H*,9X,'CONSTANT INITIAL C
     6ONCENTRATION (CI)',36X,1H*/11X,1H*,9X,'INPUT CONCENTRATION = CO (T
     7.LE.TO)',37X,1H*/11X,1H*,29X,'=  0 (T.GT.TO)',37X,1H*/11X,1H*,80X,
     81H*/11X,1H*,20A4,1H*/11X,1H*,80X,1H*/11X,82(1H*))
 1003 FORMAT(8F10.0)
 1004 FORMAT(//11X,'INPUT PARAMETERS'/11X,16(1H=)//11X,'V =',F12.4,15X,'
     1D =',F12.4/11X,'R =',F12.4,15X,'TO =',F11.4/11X,'DZERO =',F8.4,15X
     2,'CI =',F11.4/11X,'DONE =',F9.4,15X,'CO =',F11.5/11X,'TOL =',F10.5
     3)
 1005 FORMAT(///11X,'DISTANCE',11X,'TIME',7X,'PORE VOLUME',6X,'CONCENTRA
     1TION',3X,'NUMBER'/14X,'(X)',13X,'(T)',11X,'(VVO)',14X,'(C)',7X,'OF
     2 TERMS')
 1006 FORMAT(4X,3(5X,F10.4),8X,F10.4,7X,I4,F10.4)
      STOP
      END
```

EIGEN3

```
      SUBROUTINE EIGEN3(P)
C
C     PURPOSE: TO CALCULATE THE EIGENVALUES
C
      IMPLICIT REAL*8 (A-H,C-Z)
      COMMON G(20)
      BETA=0.1
      DO 4 I=1,20
      J=0
    1 J=J+1
      IF(J.GT.15) GO TO 3
      DELTA=-0.2*(-0.5)**J
    2 BET2=BETA
      BETA=BETA+DELTA
      A=BET2*DCOS(BET2)+(0.25*P-BET2**2/P)*DSIN(BET2)
      B=BETA*DCOS(BETA)+(0.25*P-BETA**2/P)*DSIN(BETA)
      IF(A*B)1,3,2
    3 G(I)=(BET2*B-BETA*A)/(B-A)
    4 BETA=BETA+0.2
      WRITE(6,1000) (G(I),I=1,20)
 1000 FORMAT(//11X,'CALCULATED EIGENVALUES'/11X,22(1H=)/(8X,5F12.6/))
      RETURN
      END
```

```
      SUBROUTINE CONS(C,V,D,DCNE,X,T,XL,TOL,I,M)
C
C     PURPOSE: TO CALCULATE CONCENTRATION C
C
      IMPLICIT REAL*8 (A-H,C-Z)
      COMMON G(20)
      I=0
      E=0.0
      U=V*DSQRT(1.+4.*DONE*D/V**2)
      P=V*XL/D
      Q=V*X/D
      PU=U*XL/D
      QU=U*X/D
      UV=(U-V)/(U+V)
      APRX=X/XL-0.9+8./P
      IF(APRX.LT.0.) GO TO 4
      IF((P.GT.100.).OR.((P-40.*V*T/XL).GT.5.)) GO TO 4
      EX=0.5*Q-0.25*V*V*T/D-DCNE*T
C
C     -----SERIES SOLUTICN-----
      C=0.0
      DO 2 J=1,10
      DC=0.0
      DC 1 K=1,2
      I=2*J+K-2
      BETA=G(I)*X/XL
      A=2.*P*G(I)*(G(I)*DCOS(BETA)+0.5*P*DSIN(BETA))
      IF(DABS(A).LT.1.D-10)A=0.0
      EXP=EX-(G(I)/XL)**2*D*T
      IF(DABS(EXP).GT.160.0) EXP=-160.
      GG=G(I)**2.+0.25*P*P
      IF(M.EQ.0) TERM=A*DEXP(EXP)/(GG*(GG+P))
      IF(M.EQ.1) TERM=A*DEXP(EXP)/((GG+P)*(GG+DONE*XL**2/D))
    1 DC=DC+TERM
      C=C+DC
      IF(DABS(DC/C).LT.TOL) GC TC 3
    2 CONTINUE
    3 IF(M.EQ.0) RETURN
      C=2.*V*(EXF(.5*(Q-QU),E)+UV*EXF(.5*(Q+QU)-PU,E))/((U+V)*(1.-UV**2*
     1EXF(-PU,E)))-C
      RETURN
C
C     ----- APPROXIMATE SOLUTICN -----
    4 S=DSQRT(4.*D*T)
      UX=2.*XL-X
      AM=(X-V*T)/S
      AP=(X+V*T)/S
      BM=(UX-V*T)/S
```

```
      EM=UX+V*T
      BP=EM/S
      CM=(UX-U*T)/S
      CP=(UX+U*T)/S
      DM=0.5*(Q-QU)
      DP=0.5*(Q+QU)
      FM=(X-U*T)/S
      FP=(X+U*T)/S
      A=0.5/BP**2
      IF(M.EQ.0) GO TO 5
      C=V/(V+U)*EXF(DM,FM)+V/(V-U)*EXF(DP,FP)+0.5*V**2/(DONE*D)*EXF(Q-DO
     1NE*T,AP)
      IF(APRX.LT.0.) RETURN
      B=-A*(1.-3.*A*(1.-5.*A*(1.-7.*A*(1.-9.*A))))
      C=(C+.5641896*V*V/DONE*DSQRT(T/D)*EXF(P-DONE*T-BP**2,E)*(V*B/D+(3.
     1+V*V/(DONE*D))*(1.+B)/EM)+V*UV/(U+V)*EXF(DP-PU,CM)-V/(UV*(U-V))*EX
     2F(DM+PU,CP))/(1.-UV**2*EXF(-PU,E))
      RETURN
    5 C=0.5*EXF(E,AM)+V*DSQRT(.3183099*T/D)*EXF(-AM*AM,E)-0.5*(1.+Q+V*V*
     1T/D)*EXF(Q,AP)
      IF(APRX.LT.0.) GO TO 6
      B=V*T/UX
      C=C+.7978846*V*UX/D*A**1.5*EXF(P-0.5/A,E)*(1.-3.*A*((1.-B)-5.*A*((
     11.-2.*B)-7.*A*((1.-3.*B)-9.*A*(1.-4.*B)))))
    6 C=(1.-C)*DEXP(-DONE*T)
      RETURN
      END
```

Table 12.--Sample output from computer C8

```
*************************************************************************
*                                                                       *
*         ONE-DIMENSIONAL CONVECTIVE-DISPERSIVE EQUATION                *
*                                                                       *
*         THIRD-TYPE BOUNDARY CONDITION                                 *
*         FINITE PROFILE                                                *
*                                                                       *
*         ZERO-ORDER PRODUCTION (DZERO)                                 *
*         FIRST-ORDER DECAY (DONE)                                      *
*         LINEAR ADSORPTION (R)                                         *
*         CONSTANT INITIAL CONCENTRATION (CI)                           *
*         INPUT CONCENTRATION = CO (T.LE.TO)                            *
*                             =  0 (T.GT.TO)                            *
*                                                                       *
*          EXAMPLE C8-1   (P=5)                                         *
*                                                                       *
*************************************************************************
```

INPUT PARAMETERS
================

V =	1.0000	D =	4.0000
R =	1.0000	TO =	1000.0000
DZERO =	0.5000	CI =	0.0
DONE =	0.2500	CO =	1.00000
TOL =	0.00010		

CALCULATED EIGENVALUES
======================

1.861513	4.212751	6.971795	9.918596	12.947841
16.017621	19.109725	22.215276	25.329502	28.449633
31.573955	34.701357	37.831086	40.962616	44.095566
47.229657	50.364677	53.500464	56.636892	59.773860

DISTANCE (X)	TIME (T)	PORE VOLUME (VVC)	CONCENTRATION (C)	NUMBER OF TERMS
0.0	5.0000	0.0	1.2715	6
2.0000	5.0000	2.5000	1.3760	6
4.0000	5.0000	1.2500	1.4310	6
6.0000	5.0000	0.8333	1.4534	6
8.0000	5.0000	0.6250	1.4570	6
10.0000	5.0000	0.5000	1.4518	8
12.0000	5.0000	0.4167	1.4441	6
14.0000	5.0000	0.3571	1.4374	8
16.0000	5.0000	0.3125	1.4327	8
18.0000	5.0000	0.2778	1.4299	8
20.0000	5.0000	0.2500	1.4290	6

DISTANCE (X)	TIME (T)	PORE VOLUME (VVC)	CONCENTRATION (C)	NUMBER OF TERMS
0.0	10.0000	0.0	1.3661	6

2.0000	10.0000	5.0000	1.5214	6
4.0000	10.0000	2.5000	1.6312	6
6.0000	10.0000	1.6667	1.7074	6
8.0000	10.0000	1.2500	1.7589	6
10.0000	10.0000	1.0000	1.7925	6
12.0000	10.0000	0.8333	1.8136	6
14.0000	10.0000	0.7143	1.8261	6
16.0000	10.0000	0.6250	1.8330	6
18.0000	10.0000	0.5556	1.8364	6
20.0000	10.0000	0.5000	1.8375	6

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION (C)	NUMBER OF TERMS
0.0	15.0000	0.0	1.3794	6
2.0000	15.0000	7.5000	1.5423	6
4.0000	15.0000	3.7500	1.6611	6
6.0000	15.0000	2.5000	1.7474	6
8.0000	15.0000	1.8750	1.8098	6
10.0000	15.0000	1.5000	1.8546	6
12.0000	15.0000	1.2500	1.8865	6
14.0000	15.0000	1.0714	1.9087	6
16.0000	15.0000	0.9375	1.9238	6
18.0000	15.0000	0.8333	1.9329	6
20.0000	15.0000	0.7500	1.9363	6

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION (C)	NUMBER OF TERMS
0.0	20.0000	0.0	1.3815	6
2.0000	20.0000	10.0000	1.5456	6
4.0000	20.0000	5.0000	1.6659	4
6.0000	20.0000	3.3333	1.7540	4
8.0000	20.0000	2.5000	1.8185	4
10.0000	20.0000	2.0000	1.8656	6
12.0000	20.0000	1.6667	1.8999	4
14.0000	20.0000	1.4286	1.9245	4
16.0000	20.0000	1.2500	1.9417	4
18.0000	20.0000	1.1111	1.9525	6
20.0000	20.0000	1.0000	1.9565	6

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION (C)	NUMBER OF TERMS
0.0	25.0000	0.0	1.3819	4
2.0000	25.0000	12.5000	1.5461	4
4.0000	25.0000	6.2500	1.6667	4
6.0000	25.0000	4.1667	1.7552	4
8.0000	25.0000	3.1250	1.8200	4
10.0000	25.0000	2.5000	1.8676	4
12.0000	25.0000	2.0833	1.9023	4
14.0000	25.0000	1.7857	1.9274	4
16.0000	25.0000	1.5625	1.9450	4
18.0000	25.0000	1.3889	1.9561	4
20.0000	25.0000	1.2500	1.9603	4

```
*****************************************************************************
*                                                                           *
*        ONE-DIMENSIONAL CONVECTIVE-DISPERSIVE EQUATION                     *
*                                                                           *
*        THIRD-TYPE BOUNDARY CONDITION                                      *
*        FINITE PROFILE                                                     *
*                                                                           *
*        ZERO-ORDER PRODUCTION (DZERO)                                      *
*        FIRST-ORDER DECAY (DONE)                                           *
*        LINEAR ADSORPTION (R)                                              *
*        CONSTANT INITIAL CONCENTRATION (CI)                                *
*        INPUT CONCENTRATION = CO (T.LE.TO)                                 *
*                            =  0 (T.GT.TO)                                 *
*                                                                           *
*         EXAMPLE C8-2                                                      *
*                                                                           *
*****************************************************************************
```

INPUT PARAMETERS
================

V = 25.0000	D = 37.5000
R = 3.0000	TO = 5.0000
DZERO = 0.5000	CI = 0.0
DONE = 0.2500	CO = 1.00000
TOL = 0.00010	

CALCULATED EIGENVALUES
======================

2.964207	5.931010	8.902794	11.881558	14.868811
17.865546	20.872271	23.889085	26.915772	29.951892
32.996868	36.050045	39.110745	42.178296	45.252056
48.331425	51.415853	54.504837	57.597926	60.694713

DISTANCE (X)	TIME (T)	PORE VOLUME (VVC)	CONCENTRATION (C)	NUMBER OF TERMS
0.0	2.5000	0.0	1.0133	0
5.0000	2.5000	12.5000	1.0478	0
10.0000	2.5000	6.2500	1.0407	0
15.0000	2.5000	4.1667	0.9560	0
20.0000	2.5000	3.1250	0.7900	0
25.0000	2.5000	2.5000	0.6034	0
30.0000	2.5000	2.0833	0.4681	0
35.0000	2.5000	1.7857	0.4027	0
40.0000	2.5000	1.5625	0.3815	0
45.0000	2.5000	1.3889	0.3769	0
50.0000	2.5000	1.2500	0.3762	0
55.0000	2.5000	1.1364	0.3761	0
60.0000	2.5000	1.0417	0.3761	0
65.0000	2.5000	0.9615	0.3761	0
70.0000	2.5000	0.8929	0.3761	0
75.0000	2.5000	0.8333	0.3761	0
80.0000	2.5000	0.7812	0.3761	0

85.0000	2.5000	0.7353	0.3761	0
90.0000	2.5000	0.6944	0.3761	0
95.0000	2.5000	0.6579	0.3761	0
100.0000	2.5000	0.6250	0.3761	0

DISTANCE (X)	TIME (T)	PORE VOLUME (VVO)	CONCENTRATION (C)	NUMBER OF TERMS
0.0	5.0000	0.0	1.0146	0
5.0000	5.0000	25.0000	1.0617	0
10.0000	5.0000	12.5000	1.1059	0
15.0000	5.0000	8.3333	1.1452	0
20.0000	5.0000	6.2500	1.1745	0
25.0000	5.0000	5.0000	1.1849	0
30.0000	5.0000	4.1667	1.1650	0
35.0000	5.0000	3.5714	1.1077	0
40.0000	5.0000	3.1250	1.0182	0
45.0000	5.0000	2.7778	0.9149	0
50.0000	5.0000	2.5000	0.8212	0
55.0000	5.0000	2.2727	0.7528	0
60.0000	5.0000	2.0833	0.7122	0
65.0000	5.0000	1.9231	0.6926	0
70.0000	5.0000	1.7857	0.6849	0
75.0000	5.0000	1.6667	0.6824	0
80.0000	5.0000	1.5625	0.6817	0
85.0000	5.0000	1.4706	0.6815	0
90.0000	5.0000	1.3889	0.6815	0
95.0000	5.0000	1.3158	0.6815	0
100.0000	5.0000	1.2500	0.6815	0

DISTANCE (X)	TIME (T)	PORE VOLUME (VVC)	CONCENTRATION (C)	NUMBER OF TERMS
0.0	7.5000	0.0	0.0303	0
5.0000	7.5000	37.5000	0.1367	0
10.0000	7.5000	18.7500	0.2737	0
15.0000	7.5000	12.5000	0.4725	0
20.0000	7.5000	9.3750	0.7296	0
25.0000	7.5000	7.5000	0.9830	0
30.0000	7.5000	6.2500	1.1652	0
35.0000	7.5000	5.3571	1.2626	0
40.0000	7.5000	4.6875	1.3027	0
45.0000	7.5000	4.1667	1.3104	0
50.0000	7.5000	3.7500	1.2946	0
55.0000	7.5000	3.4091	1.2569	0
60.0000	7.5000	3.1250	1.2014	0
65.0000	7.5000	2.8846	1.1365	0
70.0000	7.5000	2.6786	1.0725	0
75.0000	7.5000	2.5000	1.0186	0
80.0000	7.5000	2.3438	0.9792	0
85.0000	7.5000	2.2059	0.9543	0
90.0000	7.5000	2.0833	0.9405	0
95.0000	7.5000	1.9737	0.9338	0
100.0000	7.5000	1.8750	0.9314	0

DISTANCE (X)	TIME (T)	PORE VOLUME (VVC)	CONCENTRATION (C)	NUMBER OF TERMS
0.0	10.0000	0.0	0.0291	0
5.0000	10.0000	50.0000	0.1240	0
10.0000	10.0000	25.0000	0.2151	0
15.0000	10.0000	16.6667	0.3042	0
20.0000	10.0000	12.5000	0.3962	0
25.0000	10.0000	10.0000	0.4990	0
30.0000	10.0000	8.3333	0.6220	0
35.0000	10.0000	7.1429	0.7697	0
40.0000	10.0000	6.2500	0.9347	0
45.0000	10.0000	5.5556	1.0973	0
50.0000	10.0000	5.0000	1.2349	0
55.0000	10.0000	4.5455	1.3329	0
60.0000	10.0000	4.1667	1.3896	0
65.0000	10.0000	3.8462	1.4117	0
70.0000	10.0000	3.5714	1.4080	0
75.0000	10.0000	3.3333	1.3855	0
80.0000	10.0000	3.1250	1.3497	0
85.0000	10.0000	2.9412	1.3067	0
90.0000	10.0000	2.7778	1.2622	0
95.0000	10.0000	2.6316	1.2219	0
100.0000	10.0000	2.5000	1.1966	0

DISTANCE (X)	TIME (T)	PORE VOLUME (VVC)	CONCENTRATION (C)	NUMBER OF TERMS
0.0	12.5000	0.0	0.0291	0
5.0000	12.5000	62.5000	0.1239	0
10.0000	12.5000	31.2500	0.2141	0
15.0000	12.5000	20.8333	0.3000	0
20.0000	12.5000	15.6250	0.3820	0
25.0000	12.5000	12.5000	0.4608	0
30.0000	12.5000	10.4167	0.5375	0
35.0000	12.5000	8.9286	0.6143	0
40.0000	12.5000	7.8125	0.6949	0
45.0000	12.5000	6.9444	0.7833	0
50.0000	12.5000	6.2500	0.8829	0
55.0000	12.5000	5.6818	0.9939	0
60.0000	12.5000	5.2083	1.1116	0
65.0000	12.5000	4.8077	1.2270	0
70.0000	12.5000	4.4643	1.3293	0
75.0000	12.5000	4.1667	1.4098	0
80.0000	12.5000	3.9062	1.4642	0
85.0000	12.5000	3.6765	1.4932	0
90.0000	12.5000	3.4722	1.5003	0
95.0000	12.5000	3.2895	1.4908	0
100.0000	12.5000	3.1250	1.4772	0

Table 13.--Fortran listing of computer program N1 (numerical solution)

MAIN

```
C
C
C     ********************************************************************
C     *                                                                  *
C     *        ONE-DIMENSIONAL CCNVECTIVE-DISPERSIVE EQUATION       N1   *
C     *                                                                  *
C     *        NUMERICAL SOLUTION                                        *
C     *                                                                  *
C     *        LINEAR EQUILIBRIUM ADSORPTION (R)                         *
C     *        ZERO-ORDER PRODUCTION (DZERO)                             *
C     *        FIRST-ORDER DECAY (DONE)                                  *
C     *        DECAYING BOUNCARY CONDITION (DBND)                        *
C     *                                                                  *
C     ********************************************************************
C
C
      DIMENSION TITLE(20),C(200),F(200),U(200),X(200)
C
C     ---------------
      READ(5,1000) NC
      DO 14 KK=1,NC
      READ(5,1001) TITLE
      WRITE(6,1002) TITLE
C
C     ----- READ AND WRITE INPUT PARAMETERS -----
      READ(5,1003) NE,NSTEPS,KSURF,KINIT,DELX,DELT,PRDEL,DZERO,DONE,DBND
      READ(5,1004) V,D,R,CI,CA,CB,TO
      IF(KSURF.EQ.3) WRITE(6,1005)
      IF(KSURF.EQ.1) WRITE(6,1006)
      WRITE(6,1007)
      DB=ABS(DBND)
      IF(DB.LT.0.00001) CB=0
      WRITE(6,1008) NE,DELT,TO,NSTEPS,DELX,DZERO,V,CI,DONE,D,CA,DBND,R,C
     1B
C
C     ---------------
      NN=NE+1
      IF(KINIT) 1,3,5
    1 DO 2 I=1,NN
    2 C(I)=CI
      GO TO 6
    3 Y=SQRT(V*V+4.*DONE*D)
      DO 4 I=1,NN
    4 C(I)=DZERO/DONE+(CI-DZERO/DONE)*EXP((V-Y)*X(I)/(2.*D))
      GO TO 6
    5 READ(5,1004) (C(I),I=1,NN)
    6 DO 7 I=1,NN
    7 X(I)=(I-1)*DELX
```

```
      V=V*DELT/DELX
      D=D*DELT/DELX**2
      RN=(R+0.5*DELT*DONE)/6.
      RO=(R-0.5*DELT*DONE)/6.
      DZERO=DZERO*DELT
      DN=D-V*V/6.
      DO=D+V*V/6.
      EN=-0.5*DN+0.25*V+RN
      EO=0.5*DO-0.25*V+RO
      BN=-0.5*DN-0.25*V+RN
      BO=0.5*DO+0.25*V+RO
      U(1)=0.5*DN+0.25*V+2.*RN
      IF(KSURF.EQ.1) U(1)=1.0
      DN2=DN+4.*RN
      D1=-0.5*DO-0.25*V+2.*RO
      D2=-DO+4.*RO
      BND=1.0
      IF(DB.GE.0.00001) BND=(EXP(DBND*DELT)-1.)/(DBND*DELT)
      IPRINT=PRDEL/DELT
      TIME=0.0
      IF(KSURF.EQ.1) C(1)=CA+CB
      WRITE(6,1009) TIME,(X(I),C(I),I=1,NN)
C
C     ----- DYNAMIC PART OF PROGRAM -----
      DO 12 II=1,NSTEPS,IPRINT
      DO 11 JJ=1,IPRINT
      TIME=(II+JJ-1)*DELT
      IF(TIME.GT.TO) CA=0.0
      IF(TIME.GT.TO) CB=0.0
C
C     -----CONSTRUCT KNOWN VECTOR-----
      EXT=CB*EXP(-DBND*TIME)
      IF(KSURF.EQ.1) F(1)=CA+EXT
      IF(KSURF.EQ.3) F(1)=D1*C(1)+EO*C(2)+0.5*DZERO+V*(CA+BND*EXT)
      DO 8 I=2,NE
    8 F(I)=BO*C(I-1)+D2*C(I)+EO*C(I+1)+DZERO
C
C     ----- SOLVE FOR NEW VALUES ------
      R=BN/U(1)
      F(2)=F(2)-R*F(1)
      IF(KSURF.EQ.1) R=0.0
      U(2)=DN2-R*EN
      DO 9 I=3,NE
      R=BN/U(I-1)
      U(I)=DN2-R*EN
    9 F(I)=F(I)-R*F(I-1)
      C(NN)=F(NE)/(U(NE)+EN)
      DO 10 I=2,NN
```

```
      K=NN+1-I
   10 C(K)=(F(K)-EN*C(K+1))/U(K)
   11 IF(KSURF.EQ.1) C(1)=F(1)
   12 WRITE(6,1009) TIME,(X(I),C(I),I=1,NN)
   14 CONTINUE
C
C     ----------
 1000 FORMAT(I5)
 1001 FORMAT(20A4)
 1002 FORMAT(1H1,10X,82(1H*)/11X,1H*,80X,1H*/11X,1H*,9X,'ONE-DIMENSIONAL
     1 CONVECTIVE-DISPERSIVE EQUATION',25X,1H*/11X,1H*,80X,1H*/11X,1H*,9
     2X,'NUMERICAL SOLUTION',53X,1H*/11X,1H*,80X,1H*/11X,1H*,9X,'LINEAR
     3EQUILIBRIUM ADSORPTION (R)',38X,1H*/11X,1H*,9X,'ZERO-ORDER PRODUCT
     4ION (DZERO)',42X,1H*/11X,1H*,9X,'FIRST-ORDER DECAY (DONE)',47X,1H*
     5/11X,1H*,9X,'DECAYING BOUNDARY CONDITION (DBND)',37X,1H*/11X,1H*,8
     60X,1H*/11X,1H*,20A4,1H*/11X,1H*,80X,1H*)
 1003 FORMAT(4I5,6F10.0)
 1004 FORMAT(8F10.0)
 1005 FORMAT(11X,1H*,9X,'THIRD-TYPE BOUNDARY CONDITION',42X,1H*)
 1006 FORMAT(11X,1H*,9X,'FIRST-TYPE BOUNDARY CONDITION',42X,1H*)
 1007 FORMAT(11X,1H*,80X,1H*/11X,82(1H*))
 1008 FORMAT(//11X,'INPUT PARAMETERS'/11X,16(1H=)//11X,'NE =',6X,I5,15X,
     1'DELT =',F9.4,15X,'TO =',F11.4/11X,'NSTEPS =',I7,15X,'DELX =',F9.4
     2,15X,'DZERO =',F8.4/11X,'V =',F12.4,15X,'CI =',F11.4,15X,'DONE =',
     3F9.4/11X,'D =',F12.4,15X,'CA =',F11.4,15X,'DBND =',F9.4/11X,'R =',
     4F12.4,15X,'CB =',F11.4)
 1009 FORMAT(/11X,103(1H*)//11X,'CONCENTRATION AT TIME =',F10.4//3X,5(8X
     1,'DEPTH',4X,'VALUE')/(4X,5(2X,F10.2,F10.4)))
      STOP
      END
```

Table 14.--Sample output from computer program N1 (numerical solution)

```
*****************************************************************************
*                                                                           *
*        ONE-DIMENSIONAL CONVECTIVE-DISPERSIVE EQUATION                     *
*                                                                           *
*        NUMERICAL SOLUTION                                                 *
*                                                                           *
*        LINEAR EQUILIBRIUM ADSORPTION (R)                                  *
*        ZERO-ORDER PRODUCTION (DZERO)                                      *
*        FIRST-ORDER DECAY (DONE)                                           *
*        DECAYING BOUNDARY CONDITION (DBND)                                 *
*                                                                           *
*        EXAMPLE A3-1   (P=5)                                               *
*                                                                           *
*        FIRST-TYPE BOUNDARY CONDITION                                      *
*                                                                           *
*****************************************************************************

INPUT PARAMETERS
================

NE =         40               DELT =    0.2000          TO =   1000.0000
NSTEPS =    125               DELX =    0.5000          DZERO =   0.0
V =       1.0000              CI =      0.0             DONE =    0.0
D =       4.0000              CA =      1.0000          DBND =    0.0
R =       1.0000              CB =      0.0

**********************************************************************************************

CONCENTRATION AT TIME =     0.0

DEPTH    VALUE       DEPTH    VALUE       DEPTH    VALUE       DEPTH    VALUE       DEPTH    VALUE
 0.0     1.0000       0.50    0.0          1.00    0.0          1.50    0.0          2.00    0.0
 2.50    0.0          3.00    0.0          3.50    0.0          4.00    0.0          4.50    0.0
 5.00    0.0          5.50    0.0          6.00    0.0          6.50    0.0          7.00    0.0
 7.50    0.0          8.00    0.0          8.50    0.0          9.00    0.0          9.50    0.0
10.00    0.0         10.50    0.0         11.00    0.0         11.50    0.0         12.00    0.0
12.50    0.0         13.00    0.0         13.50    0.0         14.00    0.0         14.50    0.0
15.00    0.0         15.50    0.0         16.00    0.0         16.50    0.0         17.00    0.0
17.50    0.0         18.00    0.0         18.50    0.0         19.00    0.0         19.50    0.0
20.00    0.0

**********************************************************************************************

CONCENTRATION AT TIME =     5.0000

DEPTH    VALUE       DEPTH    VALUE       DEPTH    VALUE       DEPTH    VALUE       DEPTH    VALUE
 0.0     1.0000       0.50    0.9818       1.00    0.9532       1.50    0.9346       2.00    0.9019
 2.50    0.8750       3.00    0.8424       3.50    0.8089       4.00    0.7738       4.50    0.7372
 5.00    0.6995       5.50    0.6610       6.00    0.6219       6.50    0.5826       7.00    0.5433
 7.50    0.5043       8.00    0.4659       8.50    0.4285       9.00    0.3921       9.50    0.3570
10.00    0.3235      10.50    0.2917      11.00    0.2616      11.50    0.2334      12.00    0.2072
12.50    0.1830      13.00    0.1608      13.50    0.1405      14.00    0.1221      14.50    0.1056
15.00    0.0909      15.50    0.0779      16.00    0.0666      16.50    0.0567      17.00    0.0483
17.50    0.0413      18.00    0.0357      18.50    0.0313      19.00    0.0283      19.50    0.0268
20.00    0.0268

**********************************************************************************************

CONCENTRATION AT TIME =    10.0000
```

DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE
0.0	1.0000	0.50	0.9920	1.00	0.9835	1.50	0.9733	2.00	0.9628
2.50	0.9506	3.00	0.9379	3.50	0.9237	4.00	0.9087	4.50	0.8926
5.00	0.8754	5.50	0.8572	6.00	0.8380	6.50	0.8178	7.00	0.7968
7.50	0.7750	8.00	0.7524	8.50	0.7291	9.00	0.7052	9.50	0.6807
10.00	0.6559	10.50	0.6308	11.00	0.6054	11.50	0.5800	12.00	0.5546
12.50	0.5294	13.00	0.5045	13.50	0.4800	14.00	0.4561	14.50	0.4330
15.00	0.4107	15.50	0.3896	16.00	0.3697	16.50	0.3514	17.00	0.3347
17.50	0.3200	18.00	0.3075	18.50	0.2976	19.00	0.2906	19.50	0.2869
20.00	0.2869								

****

CONCENTRATION AT TIME = 15.0000

DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE
0.0	1.0000	0.50	0.9962	1.00	0.9919	1.50	0.9872	2.00	0.9819
2.50	0.9761	3.00	0.9697	3.50	0.9628	4.00	0.9553	4.50	0.9472
5.00	0.9384	5.50	0.9290	6.00	0.9190	6.50	0.9084	7.00	0.8972
7.50	0.8853	8.00	0.8729	8.50	0.8599	9.00	0.8463	9.50	0.8322
10.00	0.8176	10.50	0.8026	11.00	0.7873	11.50	0.7716	12.00	0.7556
12.50	0.7395	13.00	0.7234	13.50	0.7072	14.00	0.6912	14.50	0.6755
15.00	0.6601	15.50	0.6453	16.00	0.6312	16.50	0.6180	17.00	0.6060
17.50	0.5952	18.00	0.5861	18.50	0.5787	19.00	0.5735	19.50	0.5707
20.00	0.5707								

****

CONCENTRATION AT TIME = 20.0000

DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE
0.0	1.0000	0.50	0.9980	1.00	0.9958	1.50	0.9933	2.00	0.9905
2.50	0.9875	3.00	0.9841	3.50	0.9804	4.00	0.9764	4.50	0.9721
5.00	0.9674	5.50	0.9624	6.00	0.9570	6.50	0.9513	7.00	0.9452
7.50	0.9387	8.00	0.9319	8.50	0.9247	9.00	0.9172	9.50	0.9093
10.00	0.9012	10.50	0.8927	11.00	0.8840	11.50	0.8751	12.00	0.8660
12.50	0.8567	13.00	0.8474	13.50	0.8380	14.00	0.8287	14.50	0.8194
15.00	0.8104	15.50	0.8017	16.00	0.7934	16.50	0.7855	17.00	0.7784
17.50	0.7719	18.00	0.7665	18.50	0.7621	19.00	0.7589	19.50	0.7573
20.00	0.7573								

****

CONCENTRATION AT TIME = 25.0000

DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE
0.0	1.0000	0.50	0.9989	1.00	0.9977	1.50	0.9964	2.00	0.9949
2.50	0.9932	3.00	0.9914	3.50	0.9894	4.00	0.9872	4.50	0.9849
5.00	0.9823	5.50	0.9796	6.00	0.9766	6.50	0.9735	7.00	0.9702
7.50	0.9666	8.00	0.9629	8.50	0.9589	9.00	0.9548	9.50	0.9504
10.00	0.9459	10.50	0.9413	11.00	0.9364	11.50	0.9315	12.00	0.9264
12.50	0.9212	13.00	0.9160	13.50	0.9108	14.00	0.9056	14.50	0.9004
15.00	0.8953	15.50	0.8904	16.00	0.8858	16.50	0.8814	17.00	0.8773
17.50	0.8737	18.00	0.8706	18.50	0.8681	19.00	0.8664	19.50	0.8654
20.00	0.8654								

```
*******************************************************************************
*                                                                             *
*         ONE-DIMENSIONAL CONVECTIVE-DISPERSIVE EQUATION                      *
*                                                                             *
*         NUMERICAL SOLUTION                                                  *
*                                                                             *
*         LINEAR EQUILIBRIUM ADSORPTION (R)                                   *
*         ZERO-ORDER PRODUCTION (DZERO)                                       *
*         FIRST-ORDER DECAY (DONE)                                            *
*         DECAYING BOUNDARY CONDITION (DBND)                                  *
*                                                                             *
*         EXAMPLE B14-1                                                       *
*                                                                             *
*         THIRD-TYPE BOUNDARY CONDITION                                       *
*                                                                             *
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INPUT PARAMETERS
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NE =	40	DELT =	0.1000	TO =	1000.0000
NSTEPS =	125	DELX =	2.5000	DZERO =	0.5000
V =	25.0000	CI =	0.0	DONE =	0.0
D =	37.5000	CA =	0.0	DBND =	0.2500
R =	3.0000	CB =	10.0000		

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CONCENTRATION AT TIME = 0.0

DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE
0.0	0.0	2.50	0.0	5.00	0.0	7.50	0.0	10.00	0.0
12.50	0.0	15.00	0.0	17.50	0.0	20.00	0.0	22.50	0.0
25.00	0.0	27.50	0.0	30.00	0.0	32.50	0.0	35.00	0.0
37.50	0.0	40.00	0.0	42.50	0.0	45.00	0.0	47.50	0.0
50.00	0.0	52.50	0.0	55.00	0.0	57.50	0.0	60.00	0.0
62.50	0.0	65.00	0.0	67.50	0.0	70.00	0.0	72.50	0.0
75.00	0.0	77.50	0.0	80.00	0.0	82.50	0.0	85.00	0.0
87.50	0.0	90.00	0.0	92.50	0.0	95.00	0.0	97.50	0.0
100.00	0.0								

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CONCENTRATION AT TIME = 2.5000

DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE
0.0	5.6314	2.50	6.0918	5.00	6.5153	7.50	6.8443	10.00	7.0058
12.50	6.9274	15.00	6.5612	17.50	5.9075	20.00	5.0253	22.50	4.0229
25.00	3.0287	27.50	2.1557	30.00	1.4732	32.50	0.9977	35.00	0.7032
37.50	0.5420	40.00	0.4646	42.50	0.4323	45.00	0.4209	47.50	0.4176
50.00	0.4168	52.50	0.4167	55.00	0.4167	57.50	0.4167	60.00	0.4167
62.50	0.4167	65.00	0.4167	67.50	0.4167	70.00	0.4167	72.50	0.4167
75.00	0.4167	77.50	0.4167	80.00	0.4167	82.50	0.4167	85.00	0.4167
87.50	0.4167	90.00	0.4167	92.50	0.4167	95.00	0.4167	97.50	0.4167
100.00	0.4167								

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CONCENTRATION AT TIME = 5.0000

DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE
0.0	3.0357	2.50	3.3312	5.00	3.6457	7.50	3.9792	10.00	4.3305
12.50	4.6959	15.00	5.0687	17.50	5.4376	20.00	5.7861	22.50	6.0926
25.00	6.3309	27.50	6.4737	30.00	6.4958	32.50	6.3787	35.00	6.1158
37.50	5.7144	40.00	5.1972	42.50	4.5993	45.00	3.9636	47.50	3.3342
50.00	2.7500	52.50	2.2399	55.00	1.8199	57.50	1.4935	60.00	1.2539
62.50	1.0880	65.00	0.9795	67.50	0.9127	70.00	0.8740	72.50	0.8529
75.00	0.8422	77.50	0.8371	80.00	0.8348	82.50	0.8338	85.00	0.8335
87.50	0.8334	90.00	0.8333	92.50	0.8333	95.00	0.8333	97.50	0.8333
100.00	0.8333								

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CONCENTRATION AT TIME = 7.5000

DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE
0.0	1.6389	2.50	1.8207	5.00	2.0132	7.50	2.2174	10.00	2.4340
12.50	2.6641	15.00	2.9084	17.50	3.1675	20.00	3.4418	22.50	3.7311
25.00	4.0343	27.50	4.3491	30.00	4.6715	32.50	4.9954	35.00	5.3124
37.50	5.6117	40.00	5.8800	42.50	6.1026	45.00	6.2641	47.50	6.3503
50.00	6.3494	52.50	6.2541	55.00	6.0628	57.50	5.7805	60.00	5.4191
62.50	4.9959	65.00	4.5326	67.50	4.0528	70.00	3.5794	72.50	3.1327
75.00	2.7285	77.50	2.3772	80.00	2.0837	82.50	1.8476	85.00	1.6649
87.50	1.5287	90.00	1.4310	92.50	1.3636	95.00	1.3187	97.50	1.2898
100.00	1.2898								

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CONCENTRATION AT TIME = 10.0000

DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE
0.0	0.8912	2.50	1.0117	5.00	1.1380	7.50	1.2706	10.00	1.4099
12.50	1.5565	15.00	1.7111	17.50	1.8741	20.00	2.0464	22.50	2.2286
25.00	2.4214	27.50	2.6255	30.00	2.8415	32.50	3.0700	35.00	3.3112
37.50	3.5651	40.00	3.8310	42.50	4.1077	45.00	4.3930	47.50	4.6834
50.00	4.9743	52.50	5.2597	55.00	5.5319	57.50	5.7823	60.00	6.0011
62.50	6.1782	65.00	6.3039	67.50	6.3694	70.00	6.3683	72.50	6.2965
75.00	6.1536	77.50	5.9429	80.00	5.6716	82.50	5.3498	85.00	4.9907
87.50	4.6088	90.00	4.2191	92.50	3.8358	95.00	3.4720	97.50	3.1540
100.00	3.1540								

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CONCENTRATION AT TIME = 12.5000

DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE	DEPTH	VALUE
0.0	0.4910	2.50	0.5787	5.00	0.6696	7.50	0.7638	10.00	0.8616
12.50	0.9633	15.00	1.0693	17.50	1.1798	20.00	1.2953	22.50	1.4162
25.00	1.5428	27.50	1.6758	30.00	1.8155	32.50	1.9625	35.00	2.1173
37.50	2.2807	40.00	2.4530	42.50	2.6350	45.00	2.8271	47.50	3.0299
50.00	3.2436	52.50	3.4683	55.00	3.7037	57.50	3.9494	60.00	4.2039
62.50	4.4656	65.00	4.7316	67.50	4.9985	70.00	5.2618	72.50	5.5160
75.00	5.7548	77.50	5.9715	80.00	6.1587	82.50	6.3092	85.00	6.4162
87.50	6.4739	90.00	6.4781	92.50	6.4265	95.00	6.3216	97.50	6.1898
100.00	6.1898								