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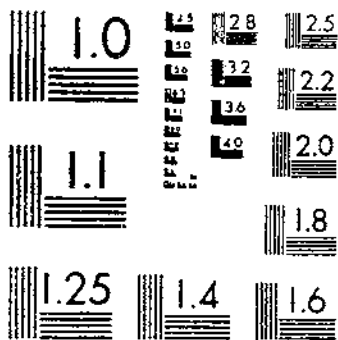
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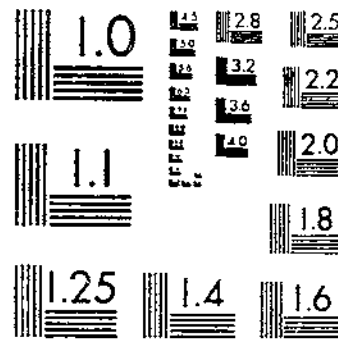
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ANALYTICAL SOLUTIONS OF THE ONE-DIMENSIONAL CONVECTIVE-DISPERSIVE SOLUTE
VAN GENUCHTEN, H. ALYES, W. J. — OF 2

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

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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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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 conjunction 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

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

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

$$s = k c \quad [2]$$

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

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

where the retardation factor R is given by

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

and with the new rate coefficients μ and γ given by

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

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

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

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

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

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

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

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

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

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

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

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

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

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:

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

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

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

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 | | | | |
|---|--|-------------------|----------------------------|---------------------------------------|
| $R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x}$ | | | | |
| Upper boundary condition | | | | |
| Case | Initial condition $f(x)^1$ | Type ² | $g(t)^3$ | 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 | $\begin{cases} C_1 & (0 < x < x_1) \\ C_2 & (x > x_1) \end{cases}$ | 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 | | | | |
|---|-------------------------------|-------------------|----------------------------|---------------------------------------|
| $R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x}$ | | | | |
| Upper boundary condition | | | | |
| Case | Initial condition $f(x)^1$ | Type ² | $g(t)^3$ | Lower boundary condition ⁴ |
| A7 | $C_1 + C_2 e^{-\alpha x}$ | 1 | C_0 (pulse) ⁵ | --do-- |
| A8 | --do-- | 3 | --do-- | --do-- |
| A9 | C_1 | 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 | | | | |
|--|--------------------|---|----------------------------|----------------|
| $R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} + \gamma$ | | | | |
| B1 | NA ⁶ | 1 | C_0 | Semi-inifite. |
| B2 | --do-- | 3 | --do-- | --do-- |
| B3 | --do-- | 1 | --do-- | Finite. |
| B4 | --do-- | 3 | --do-- | --do-- |
| B5 | C_1 | 1 | C_0 (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_1 | 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 | | Lower boundary condition ⁴ |
| | | Type ² | $g(t)^3$ | |
| C1 | NA ⁶ | 1 | C_0 | Semi-infinite. |
| C2 | --do-- | 3 | --do-- | --do-- |
| C3 | --do-- | 1 | --do-- | Finite. |
| C4 | --do-- | 3 | --do-- | --do-- |
| C5 | C_i | 1 | C_0 (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].

⁴Equation [10a] or [10c] for a semi-infinite system; equation [10b] for a finite system.

⁵Indicates a pulse-type application:

$$g(t) = \begin{cases} C_0 & (0 < t < t_0) \\ 0 & (t > t_0) \end{cases}$$

⁶Not applicable; steady-state solution.

⁷Steady-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

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

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

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

or

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

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

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

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

$$c(x,0) = C_1$$

$$c(0,t) = \begin{cases} C_0 & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

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

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

$$c(x,t) = \begin{cases} C_1 + (C_0 - C_1) A(x,t) & 0 < t < t_0 \\ C_1 + (C_0 - C_1) A(x,t) - C_0 A(x,t-t_0) & t > t_0 \end{cases}$$

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

$$c(x,0) = C_1$$

$$\left. \left(-D \frac{\partial c}{\partial x} + vc \right) \right|_{x=0} = \begin{cases} vC_0 & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

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

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

$$c(x,t) = \begin{cases} C_1 + (C_0 - C_1) A(x,t) & 0 < t < t_0 \\ C_1 + (C_0 - C_1) A(x,t) - C_0 A(x, t-t_0) & t > t_0 \end{cases}$$

where

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

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

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

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

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

Analytical Solution (Cleary and Adrian 1973).

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

where

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

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

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

Approximate Solution

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

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

$$c(x, 0) = C_1$$

$$\left. \left(-D \frac{\partial c}{\partial x} + vc \right) \right|_{x=0} = \begin{cases} vC_0 & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

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

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

$$c(x, t) = \begin{cases} C_1 + (C_0 - C_1) A(x, t) & 0 < t < t_0 \\ C_1 + (C_0 - C_1) A(x, t) - C_0 A(x, t - t_0) & t > t_0 \end{cases}$$

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

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

Approximate Solution (Brenner 1962)

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

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

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

$$c(0,t) = \begin{cases} C_0 & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

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

Analytical Solution

$$c(x,t) =$$

$$\begin{cases} C_2 + (C_1 - C_2) A(x,t) + (C_0 - C_1) B(x,t) & 0 < t < t_0 \\ C_2 + (C_1 - C_2) A(x,t) + (C_0 - C_1) B(x,t) - C_0 B(x, t - t_0) & t > t_0 \end{cases}$$

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

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

$$\left. \left(-D \frac{\partial c}{\partial x} + vc \right) \right|_{x=0} = \begin{cases} vC_0 & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

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

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

$$c(x,t) =$$

$$\begin{cases} C_2 + (C_1 - C_2) A(x,t) + (C_0 - C_1) B(x,t) & 0 < t < t_0 \\ C_2 + (C_1 - C_2) A(x,t) + (C_0 - C_1) B(x,t) - C_0 B(x, t-t_0) & t > t_0 \end{cases}$$

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

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

$$c(0, t) = \begin{cases} C_0 & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

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

Analytical Solution

$$c(x, t) =$$

$$\begin{cases} C_1 + (C_0 - C_1) A(x, t) + C_2 B(x, t) & 0 < t < t_0 \\ C_1 + (C_0 - C_1) A(x, t) + C_2 B(x, t) - C_0 A(x, t - t_0) & t > t_0 \end{cases}$$

where

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

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

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

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

$$\left(-D \frac{\partial c}{\partial x} + vc\right) \Big|_{x=0} = \begin{cases} vC_0 & 0 < t \leq t_0 \\ 0 & t > t_0 \end{cases}$$

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

Analytical Solution

$$c(x,t) =$$

$$\begin{cases} C_1 + (C_0 - C_1) A(x,t) + C_2 B(x,t) & 0 < t \leq t_0 \\ C_1 + (C_0 - C_1) A(x,t) + C_2 B(x,t) - C_0 A(x, t-t_0) & t > t_0 \end{cases}$$

where

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

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

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

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

All. 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

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

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

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

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

and

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

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:

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

where

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

Approximate Solution

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

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

where

$$\begin{aligned} B_3(x,t) = & \frac{1}{2} \exp\left[\frac{(v-y)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - yt}{2(DRt)^{1/2}}\right] \\ & + \frac{1}{2} \exp\left[\frac{(v+y)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + yt}{2(DRt)^{1/2}}\right] \\ & + \frac{(y-v)}{2(y+v)} \exp\left[\frac{(v+y)x - 2yL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) - yt}{2(DRt)^{1/2}}\right] \end{aligned}$$

$$\begin{aligned}
& + \frac{(y+v)}{2(y-v)} \exp\left[\frac{(v-y)x + 2yL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) + yt}{2(DRt)^{1/2}}\right] \\
& + \frac{v^2}{2\lambda DR} \exp\left(\frac{vL}{D} + \lambda t\right) \operatorname{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]
\end{aligned}$$

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

and

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

A12. Governing Equation

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

Initial and Boundary Conditions

$$c(x, 0) = C_1$$

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

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

Analytical Solution

$$c(x, t) = C_1 + (C_a - C_1) A(x, t) + C_b B(x, t)$$

where

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

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

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

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

and

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

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 $B_1(x)$ 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:

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

where

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

Approximate Solution

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

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

where

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

$$\begin{aligned}
& + \left(\frac{v}{v-y}\right) \exp\left[\frac{(v+y)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + yt}{2(DRt)^{1/2}}\right] \\
& - \frac{v^2}{2\lambda DR} \exp\left(\frac{vx}{D} + \lambda t\right) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right] \\
& - \frac{v^2}{2\lambda DR} \left[\frac{v(2L-x)}{D} + \frac{v^2 t}{DR} + 3 - \frac{v^2}{\lambda DR}\right] \exp\left(\frac{vL}{D} + \lambda t\right) \operatorname{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right] \\
& + \frac{v^3}{\lambda DR} \left(\frac{t}{\pi DR}\right)^{1/2} \exp\left[\frac{vL}{D} + \lambda t - \frac{R}{4Dt} \left(2L-x + \frac{vt}{R}\right)^2\right] \\
& + \frac{v(y-v)}{(y+v)^2} \exp\left[\frac{(v+y)x - 2yL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) - yt}{2(DRt)^{1/2}}\right] \\
& - \frac{v(y+v)}{(y-v)^2} \exp\left[\frac{(v-y)x + 2yL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) + yt}{2(DRt)^{1/2}}\right] \\
B_4(x) & = 1 - \frac{(y-v)^2}{(y+v)^2} \exp(-yL/D)
\end{aligned}$$

B. Solutions for Zero-order Production Only

B1. Governing Equation (Steady-state) $D \frac{d^2 c}{dx^2} - v \frac{dc}{dx} + \gamma = 0$

Boundary Conditions

$$c(0) = C_0$$

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

Analytical Solution

$$c(x) = C_0 + \frac{\gamma x}{v}$$

B2. Governing
Equation
(Steady-state)

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

Boundary Conditions

$$\left(-D \frac{dc}{dx} + vc\right) \Big|_{x=0} = vC_0$$

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

Analytical Solution

$$c(x) = C_0 + \frac{\gamma(vx+D)}{v^2}$$

B3. Governing
Equation
(Steady-state)

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

Boundary Conditions

$$c(0) = C_0$$

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

Analytical Solution

$$c(x) = C_0 + \sum_{m=1}^{\infty} \frac{2\beta_m \sin\left(\frac{\beta_m x}{L}\right) \frac{\gamma L^2}{D} \exp\left(\frac{vx}{2D}\right)}{\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2 + \frac{vL}{2D}\right] \left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2\right]}$$

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

$$c(x) = C_0 + \frac{\gamma x}{v} + \frac{\gamma D}{2} \left\{ \exp\left(-\frac{vL}{D}\right) - \exp\left[\frac{(x-L)v}{D}\right] \right\}$$

B4. Governing Equation
(Steady-state)

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

Boundary Conditions

$$\left(-D \frac{dc}{dx} + vc\right) \Big|_{x=0} = vC_0$$

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

Analytical Solution

$$c(x) = C_0 + \sum_{m=1}^{\infty} \frac{\left(\frac{2vL}{D}\right) \left(\frac{\gamma L^2}{D}\right) \beta_m \left[\beta_m \cos\left(\frac{\beta_m x}{L}\right) + \frac{vL}{2D} \sin\left(\frac{\beta_m x}{L}\right)\right] \exp\left(\frac{vx}{2D}\right)}{\left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2 + \frac{vL}{D}\right] \left[\beta_m^2 + \left(\frac{vL}{2D}\right)^2\right]}$$

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

$$c(x) = C_0 + \frac{\gamma x}{v} + \frac{\gamma D}{v^2} \left\{1 - \exp\left[\frac{v(x-L)}{D}\right]\right\}$$

B5. Governing Equation

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

Initial and Boundary Conditions

$$c(x, 0) = C_1$$

$$c(0, t) = \begin{cases} C_0 & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

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

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

$$c(x, t) = \begin{cases} C_1 + (C_0 - C_1) A(x, t) + B(x, t) & 0 < t < t_0 \\ C_1 + (C_0 - C_1) A(x, t) + B(x, t) - C_0 A(x, t - t_0) & t > t_0 \end{cases}$$

where

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

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

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

$$c(x,0) = C_1$$

$$\left(-D \frac{\partial c}{\partial x} + vc\right) \Big|_{x=0} = \begin{cases} vC_0 & 0 < t \leq t_0 \\ 0 & t > t_0 \end{cases}$$

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

Analytical Solution (van Genuchten 1981)

$$c(x,t) = \begin{cases} C_1 + (C_0 - C_1) A(x,t) + B(x,t) & 0 < t \leq t_0 \\ C_1 + (C_0 - C_1) A(x,t) + B(x,t) - C_0 A(x, t-t_0) & t > t_0 \end{cases}$$

where

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

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

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

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

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

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

Analytical Solution

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

where

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

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

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

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

and

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

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):

$$B_1(x) = \frac{Yx}{v} + \frac{YD}{2} \left\{ \exp\left(-\frac{vL}{D}\right) - \exp\left[\frac{(x-L)v}{D}\right] \right\}$$

Approximate Solution:

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

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

B8. Governing Equations

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

Initial and Boundary Conditions

$$c(x, 0) = C_1$$

$$\left. \left(-D \frac{\partial c}{\partial x} + vc \right) \right|_{x=0} = \begin{cases} C_0 & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

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

Analytical Solution

$$c(x, t) = \begin{cases} C_1 + (C_0 - C_1) A(x, t) + B(x, t) & 0 < t < t_0 \\ C_1 + (C_0 - C_1) A(x, t) + B(x, t) - C_0 A(x, t - t_0) & t > t_0 \end{cases}$$

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

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

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 $B_1(x)$, 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:

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

Approximate Solution

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

$$\begin{aligned}
B(x,t) = \frac{Y}{R} \left\{ t + \frac{1}{2v} \left(Rx - vt + \frac{DR}{v} \right) \operatorname{erfc} \left[\frac{Rx - vt}{2(DRt)^{1/2}} \right] \right. \\
- \left(\frac{t}{4\pi DR} \right)^{1/2} \left(Rx + vt + \frac{2DR}{v} \right) \exp \left[- \frac{(Rx - vt)^2}{4DRt} \right] \\
+ \left[\frac{t}{2} - \frac{DR}{2v^2} + \frac{(Rx + vt)^2}{4DR} \right] \exp(vx/D) \operatorname{erfc} \left[\frac{Rx + vt}{2(DRt)^{1/2}} \right] \\
- \frac{DR}{2v^2} \exp \left[\frac{v(x-L)}{D} \right] \operatorname{erfc} \left[\frac{R(2L-x) - vt}{2(DRt)^{1/2}} \right] \\
+ \frac{DR}{2v^2} \left[1 - \frac{v(2L-x)}{2D} + \frac{v^2}{2D^2} \left(2L-x + \frac{vt}{R} \right) \left(2L-x + \frac{3vt}{R} \right) \right. \\
\left. + \frac{v^3}{6D^3} \left(2L-x + \frac{vt}{R} \right)^3 \right] \exp(vL/D) \operatorname{erfc} \left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}} \right] \\
- \frac{R}{v} \left[-1 + \frac{v}{2D} \left(2L-x + \frac{7vt}{3R} \right) + \frac{v^2}{6D^2} \left(2L-x + \frac{vt}{R} \right)^2 \right] \\
\left. \left(\frac{Dt}{\pi R} \right)^{1/2} \exp \left[\frac{vL}{D} - \frac{R}{4Dt} \left(2L-x + \frac{vt}{R} \right)^2 \right] \right\}
\end{aligned}$$

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

$$c(x, 0) = C_1 + \frac{\gamma x}{v}$$

$$c(0, t) = \begin{cases} C_0 & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

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

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

$$c(x, t) = \begin{cases} C_1 + \frac{\gamma x}{v} + (C_0 - C_1) A(x, t) & 0 < t < t_0 \\ C_1 + \frac{\gamma x}{v} + (C_0 - C_1) A(x, t) - C_0 A(x, t - t_0) & t > t_0 \end{cases}$$

where

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

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

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

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

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

Analytical Solution

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

where

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

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

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

$$= C_1 + \frac{\gamma x}{v} + \frac{\gamma D}{v^2} \left\{ \exp\left(-\frac{vL}{D}\right) - \exp\left[\frac{v(x-L)}{D}\right] \right\}$$

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

Boundary Conditions

$$c(0,t) = \begin{cases} C_0 & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

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

Analytical Solution

$$c(x,t) = \begin{cases} A(x) + (C_0 - C_1) B(x,t) & 0 < t < t_0 \\ A(x) + (C_0 - C_1) B(x,t) - C_0 B(x,t-t_0) & t > t_0 \end{cases}$$

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

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

The eigenvalues β_m are the positive roots of the equation

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

Approximate Solution

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

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

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

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

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

Boundary Conditions

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

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

Analytical Solution

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

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

$$B(x,t) =$$

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

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

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

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

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

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

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

and

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

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

$$c(x,0) = C_1$$

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

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

Analytical Solution

$$c(x,t) = C_1 + (C_a - C_1) A(x,t) + C_b B(x,t) + F(x,t)$$

where

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

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

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

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

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

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

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

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

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

and

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

Approximate Solution

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

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

$$\begin{aligned}
 B_3(x,t) &= \frac{1}{2} \exp \left[\frac{(v-y)x}{2D} \right] \operatorname{erfc} \left[\frac{Rx - yt}{2(DRt)^{1/2}} \right] \\
 &+ \frac{1}{2} \exp \left[\frac{(v+y)x}{2D} \right] \operatorname{erfc} \left[\frac{Rx + yt}{2(DRt)^{1/2}} \right] \\
 &+ \frac{(y-v)}{2(y+v)} \exp \left[\frac{(v+y)x - 2yL}{2D} \right] \operatorname{erfc} \left[\frac{R(2L-x) - yt}{2(DRt)^{1/2}} \right] \\
 &+ \frac{(y+v)}{2(y-v)} \exp \left[\frac{(v-y)x + 2yL}{2D} \right] \operatorname{erfc} \left[\frac{R(2L-x) + yt}{2(DRt)^{1/2}} \right] \\
 &+ \frac{v^2}{2\lambda DR} \exp \left(\frac{vL}{D} + \lambda t \right) \operatorname{erfc} \left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}} \right]
 \end{aligned}$$

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

and

$$\begin{aligned}
 F(x,t) &= \frac{Y}{R} \left\{ t + \frac{(Rx-vt)}{2v} \operatorname{erfc} \left[\frac{Rx - vt}{2(DRt)^{1/2}} \right] \right. \\
 &\quad \left. - \frac{(Rx+vt)}{2v} \exp(vx/D) \operatorname{erfc} \left[\frac{Rx + vt}{2(DRt)^{1/2}} \right] \right\}
 \end{aligned}$$

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

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

$$c(x,0) = C_1$$

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

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

Analytical Solution

$$c(x,t) = C_1 + (C_a - C_1) A(x,t) + C_b B(x,t) + F(x,t)$$

where

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

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

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

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

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

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

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

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

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

and

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

Approximate Solution

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

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

$$\begin{aligned}
 B_3(x,t) = & \left(\frac{v}{v+y} \right) \exp \left[\frac{(v-y)x}{2D} \right] \operatorname{erfc} \left[\frac{Rx - yt}{2(DRt)^{1/2}} \right] \\
 & + \left(\frac{v}{v-y} \right) \exp \left[\frac{(v+y)x}{2D} \right] \operatorname{erfc} \left[\frac{Rx + yt}{2(DRt)^{1/2}} \right] \\
 & - \frac{v^2}{2\lambda DR} \exp \left(\frac{vx}{D} + \lambda t \right) \operatorname{erfc} \left[\frac{Rx + vt}{2(DRt)^{1/2}} \right] \\
 & - \frac{v^2}{2\lambda DR} \left[\frac{v(2L-x)}{D} + \frac{v^2 t}{DR} + 3 - \frac{v^2}{\lambda DR} \right] \exp \left(\frac{vL}{D} + \lambda t \right) \operatorname{erfc} \left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}} \right] \\
 & + \frac{v^3}{\lambda DR} \left(\frac{t}{\pi DR} \right)^{1/2} \exp \left[\frac{vL}{D} + \lambda t - \frac{R}{4Dt} \left(2L - x + \frac{vt}{R} \right)^2 \right] \\
 & + \frac{v(y-v)}{(y+v)^2} \exp \left[\frac{(v+y)x - 2yL}{2D} \right] \operatorname{erfc} \left[\frac{R(2L-x) - yt}{2(DRt)^{1/2}} \right] \\
 & - \frac{v(y+v)}{(y-v)^2} \exp \left[\frac{(v-y)x + 2yL}{2D} \right] \operatorname{erfc} \left[\frac{R(2L-x) + yt}{2(DRt)^{1/2}} \right]
 \end{aligned}$$

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

and

$$\begin{aligned}
 F(x,t) = \frac{Y}{R} \left\{ t + \frac{1}{2v} \left(Rx - vt + \frac{DR}{v} \right) \operatorname{erfc} \left[\frac{Rx - vt}{2(DRt)^{1/2}} \right] \right. \\
 - \left(\frac{t}{4\pi DR} \right)^{1/2} \left(Rx + vt + \frac{2DR}{v} \right) \exp \left[- \frac{(Rx - vt)^2}{4DRt} \right] \\
 + \left[\frac{t}{2} - \frac{DR}{2v^2} + \frac{(Rx + vt)^2}{4DR} \right] \exp(vx/D) \operatorname{erfc} \left[\frac{Rx + vt}{2(DRt)^{1/2}} \right] \\
 - \frac{DR}{2v^2} \exp \left[\frac{v(x-L)}{D} \right] \operatorname{erfc} \left[\frac{R(2L-x) - vt}{2(DRt)^{1/2}} \right] \\
 + \frac{DR}{2v^2} \left[1 - \frac{v(2L-x)}{2D} + \frac{v^2}{2D^2} (2L-x + \frac{vt}{R})(2L-x + \frac{3vt}{R}) \right. \\
 \left. + \frac{v^3}{6D^3} (2L-x + \frac{vt}{R})^3 \right] \exp(vL/D) \operatorname{erfc} \left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}} \right] \\
 - \frac{R}{v} \left[-1 + \frac{v}{2D} (2L-x + \frac{7vt}{3R}) + \frac{v^2}{6D^2} (2L-x + \frac{vt}{R})^2 \right] \\
 \left. \left(\frac{Dt}{\pi R} \right)^{1/2} \exp \left[\frac{vL}{D} - \frac{R}{4Dt} (2L-x + \frac{vt}{R})^2 \right] \right\}
 \end{aligned}$$

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

Cl. Governing Equation
(Steady-state)

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

Boundary Conditions

$$c(0) = C_0$$

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

Analytical Solution

$$c(x) = \frac{\gamma}{\mu} + (C_0 - \frac{\gamma}{\mu}) \exp\left[\frac{(v-u)x}{2D}\right]$$

where

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

C2. Governing
Equation
(Steady-state)

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

Boundary Conditions

$$\left(-D \frac{dc}{dx} + vc\right) \Big|_{x=0} = vC_0$$

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

Analytical Solution (Gershon and Nir 1969)

$$c(x) = \frac{\gamma}{\mu} + (C_0 - \frac{\gamma}{\mu}) \frac{2v}{u+v} \exp\left[\frac{(v-u)x}{2D}\right]$$

where

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

C3. Governing
Equation
(Steady-state)

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

Boundary Conditions

$$c(0) = C_0$$

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

Analytical Solution

$$c(x) = \frac{\gamma}{\mu} + (C_0 - \frac{\gamma}{\mu}) A(x)$$

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

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

C4. Governing Equation (Steady-state)

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

Boundary Conditions

$$\left(-D \frac{dc}{dx} + vc\right) \Big|_{x=0} = vC_0$$

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

Analytical Solution

$$c(x) = \frac{\gamma}{\mu} + (C_0 - \frac{\gamma}{\mu}) A(x)$$

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

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

Initial and Boundary Conditions

$$c(x,0) = C_1$$

$$c(0,t) = \begin{cases} C_0 & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

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

Analytical Solution (van Genuchten 1981; see also Bear 1972, p. 630)

$$c(x,t) =$$

$$\begin{cases} \frac{\gamma}{\mu} + (C_1 - \frac{\gamma}{\mu}) A(x,t) + (C_0 - \frac{\gamma}{\mu}) B(x,t) & 0 < t < t_0 \\ \frac{\gamma}{\mu} + (C_1 - \frac{\gamma}{\mu}) A(x,t) + (C_0 - \frac{\gamma}{\mu}) B(x,t) - C_0 B(x, t-t_0) & t > t_0 \end{cases}$$

where

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

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

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

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

$$c(x, 0) = C_1$$

$$\left. \left(-D \frac{\partial c}{\partial x} + vc \right) \right|_{x=0} = \begin{cases} vC_0 & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

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

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

$$c(x, t) =$$

$$\begin{cases} \frac{Y}{\mu} + (C_1 - \frac{Y}{\mu}) A(x, t) + (C_0 - \frac{Y}{\mu}) B(x, t) & 0 < t < t_0 \\ \frac{Y}{\mu} + (C_1 - \frac{Y}{\mu}) A(x, t) + (C_0 - \frac{Y}{\mu}) B(x, t) - C_0 B(x, t - t_0) & t > t_0 \end{cases}$$

where

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

$$\begin{aligned}
B(x,t) &= \frac{v}{(v+u)} \exp\left[\frac{(v-u)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - ut}{2(DRt)^{1/2}}\right] \\
&+ \frac{v}{(v-u)} \exp\left[\frac{(v+u)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + ut}{2(DRt)^{1/2}}\right] \\
&+ \frac{v^2}{2\mu D} \exp\left(\frac{vx}{D} - \frac{\mu t}{R}\right) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]
\end{aligned}$$

and

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

C7. Governing Equation

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

Initial and Boundary Conditions

$$c(x, 0) = C_1$$

$$c(0, t) = \begin{cases} C_0 & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

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

Analytical Solution (Selim and Mansell 1976)

$$c(x, t) =$$

$$\begin{cases} \frac{\gamma}{\mu} + (C_1 - \frac{\gamma}{\mu}) A(x, t) + (C_0 - \frac{\gamma}{\mu}) B(x, t) & 0 < t < t_0 \\ \frac{\gamma}{\mu} + (C_1 - \frac{\gamma}{\mu}) A(x, t) + (C_0 - \frac{\gamma}{\mu}) B(x, t) - C_0 B(x, t - t_0) & t > t_0 \end{cases}$$

where

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

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

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

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

and

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

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:

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

Approximate Solution

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

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

where

$$\begin{aligned}
B_3(x, t) = & \frac{1}{2} \exp\left[\frac{(v-u)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - ut}{2(DRt)^{1/2}}\right] \\
& + \frac{1}{2} \exp\left[\frac{(v+u)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + ut}{2(DRt)^{1/2}}\right] \\
& + \frac{(u-v)}{2(u+v)} \exp\left[\frac{(v+u)x - 2uL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) - ut}{2(DRt)^{1/2}}\right] \\
& + \frac{(u+v)}{2(u-v)} \exp\left[\frac{(v-u)x + 2uL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) + ut}{2(DRt)^{1/2}}\right] \\
& - \frac{v^2}{2\mu D} \exp\left(\frac{vL}{D} - \frac{\mu t}{R}\right) \operatorname{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]
\end{aligned}$$

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

and

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

C8. Governing Equation
$$K \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} - \mu c + \gamma$$

Initial and Boundary Conditions

$$c(x, 0) = C_1$$

$$\left. (-D \frac{\partial c}{\partial x} + vc) \right|_{x=0} = \begin{cases} vC_0 & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

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

Analytical Solution

$$c(x, t) =$$

$$\begin{cases} \frac{\gamma}{\mu} + (C_1 - \frac{\gamma}{\mu}) A(x, t) + (C_0 - \frac{\gamma}{\mu}) B(x, t) & 0 < t < t_0 \\ \frac{\gamma}{\mu} + (C_1 - \frac{\gamma}{\mu}) A(x, t) + (C_0 - \frac{\gamma}{\mu}) B(x, t) - C_0 B(x, t - t_0) & t > t_0 \end{cases}$$

where

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

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

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

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

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:

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

Approximate Solution

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

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

where

$$\begin{aligned}
 B_3(x,t) = & \frac{v}{(v+u)} \exp\left[-\frac{(v-u)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - ut}{2(DRt)^{1/2}}\right] \\
 & + \frac{v}{(v-u)} \exp\left[\frac{(v+u)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + ut}{2(DRt)^{1/2}}\right] \\
 & + \frac{v^2}{2\mu D} \exp\left(\frac{vx}{D} - \frac{\mu t}{R}\right) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right] \\
 & + \frac{v^2}{2\mu D} \left[\frac{v(2L-x)}{D} + \frac{v^2 t}{DR} + 3 + \frac{v^2}{\mu D} \right] \exp\left(\frac{vL}{D} - \frac{\mu t}{R}\right) \operatorname{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right] \\
 & - \frac{v^3}{\mu D} \left(\frac{t}{\pi DR}\right)^{1/2} \exp\left[\frac{vL}{D} - \frac{\mu t}{R} - \frac{R}{4Dt}(2L-x + \frac{vt}{R})^2\right] \\
 & + \frac{v(u-v)}{(u+v)^2} \exp\left[\frac{(v+u)x - 2uL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) - ut}{2(DRt)^{1/2}}\right] \\
 & - \frac{v(u+v)}{(u-v)^2} \exp\left[\frac{(v-u)x + 2uL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) + ut}{2(DRt)^{1/2}}\right] \\
 B_4(x) = & 1 - \frac{(u-v)^2}{(u+v)^2} \exp(-uL/D)
 \end{aligned}$$

and

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

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

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

$$= \frac{\gamma}{\mu} + (C_1 - \frac{\gamma}{\mu}) \exp \left[\frac{(v-u)x}{2D} \right]$$

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

$$c(0,t) = \begin{cases} C_0 & 0 < t \leq t_0 \\ 0 & t > t_0 \end{cases}$$

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

Analytical Solution

$$c(x,t) = \begin{cases} A(x) + (C_0 - C_1) B(x,t) & 0 < t \leq t_0 \\ A(x) + (C_0 - C_1) B(x,t) - C_0 B(x,t-t_0) & t > t_0 \end{cases}$$

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

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

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

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 C2).

Boundary Conditions

$$\left(-D \frac{\partial c}{\partial x} + vc\right) \Big|_{x=0} = \begin{cases} vC_0 & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

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

Analytical Solution

$$c(x,t) = \begin{cases} A(x) + (C_0 - C_i) B(x,t) & 0 < t < t_0 \\ A(x) + (C_0 - C_i) B(x,t) - C_0 B(x, t-t_0) & t > t_0 \end{cases}$$

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

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

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

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

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

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

$$= \frac{\gamma}{\mu} + (C_1 - \frac{\gamma}{\mu}) \frac{\exp[\frac{(v-u)x}{2D}] + (\frac{u-v}{u+v}) \exp[\frac{(v+u)x - 2uL}{2D}]}{[1 + (\frac{u-v}{u+v}) \exp(-uL/D)]}$$

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

$$c(0,t) = \begin{cases} C_0 & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

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

Analytical Solution

$$c(x,t) = \begin{cases} A(x) + (C_0 - C_1) B(x,t) & 0 < t < t_0 \\ A(x) + (C_0 - C_1) B(x,t) - C_0 B(x,t-t_0) & t > t_0 \end{cases}$$

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

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

$$\begin{aligned}
& + \frac{1}{2} \exp\left[\frac{(v+u)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + ut}{2(DRt)^{1/2}}\right] \\
& + \frac{(u-v)}{2(u+v)} \exp\left[\frac{(v+u)x - 2uL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) - ut}{2(DRt)^{1/2}}\right] \\
& + \frac{(u+v)}{2(u-v)} \exp\left[\frac{(v-u)x + 2uL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) + ut}{2(DRt)^{1/2}}\right] \\
& - \frac{v^2}{2\mu D} \exp\left[-\frac{vL}{D} - \frac{\mu t}{R}\right] \operatorname{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right]
\end{aligned}$$

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

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

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

$$= \frac{\gamma}{\mu} + (C_1 - \frac{\gamma}{\mu}) \frac{\exp[\frac{(v-u)x}{2D}] + (\frac{u-v}{u+v}) \exp[\frac{(v+u)x - 2uL}{2D}]}{[\frac{u+v}{2v} - \frac{(u-v)^2}{2v(u+v)} \exp(-uL/D)]}$$

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

$$\left(-D \frac{\partial c}{\partial x} + vc\right) \Big|_{x=0} = \begin{cases} vC_0 & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

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

Analytical Solution

$$c(x,t) = \begin{cases} A(x) + (C_0 - C_1) B(x,t) & 0 < t < t_0 \\ A(x) + (C_0 - C_1) B(x,t) - C_0 B(x,t-t_0) & t > t_0 \end{cases}$$

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

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

with

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

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

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:

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

Approximate Solution

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

where

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

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

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 (1974b) 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

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

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

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

and with

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

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

C14. Governing Equation

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

Initial and Boundary Conditions

$$c(x, 0) = C_1$$

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

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

Analytical Solution (see also Lindstrom and Oberhettinger 1975)

$$c(x, t) =$$

$$\begin{cases} \frac{\gamma}{\mu} + (C_1 - \frac{\gamma}{\mu}) A(x, t) + (C_a - \frac{\gamma}{\mu}) B(x, t) + C_b E(x, t) & (\mu \neq \lambda R) \\ \frac{\gamma}{\mu} + (C_1 - C_b - \frac{\gamma}{\mu}) A(x, t) + (C_a - \frac{\gamma}{\mu}) B(x, t) + C_b e^{-\lambda t} & (\mu = \lambda R) \end{cases}$$

where

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

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

$$\begin{aligned}
& + \frac{v^2}{2\mu D} \exp\left(\frac{vx}{D} - \frac{\mu t}{R}\right) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right] \\
E(x,t) = e^{-\lambda t} & \left\{ \left(\frac{v}{v+w}\right) \exp\left[\frac{(v-w)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - wt}{2(DRt)^{1/2}}\right] \right. \\
& \left. + \left(\frac{v}{v-w}\right) \exp\left[\frac{(v+w)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + wt}{2(DRt)^{1/2}}\right] \right\} \\
& + \frac{v^2}{2D(\mu - \lambda R)} \exp\left(\frac{vx}{D} - \frac{\mu t}{R}\right) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]
\end{aligned}$$

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

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

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

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

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

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

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

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

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

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

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

Approximate Solution

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

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

where

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

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

and

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

where

$$\begin{aligned} F_3(x,t) = & \frac{1}{2} \exp\left[\frac{(v-w)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - wt}{2(DRt)^{1/2}}\right] \\ & + \frac{1}{2} \exp\left[\frac{(v+w)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + wt}{2(DRt)^{1/2}}\right] \\ & + \frac{(w-v)}{2(w+v)} \exp\left[\frac{(v+w)x - 2wL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) - wt}{2(DRt)^{1/2}}\right] \\ & + \frac{(w+v)}{2(w-v)} \exp\left[\frac{(v-w)x + 2wL}{2D}\right] \operatorname{erfc}\left[\frac{R(2L-x) + wt}{2(DRt)^{1/2}}\right] \\ & - \frac{v^2}{2D(\mu - \lambda R)} \exp\left(\frac{vL}{D} - \frac{\mu t}{R} + \lambda t\right) \operatorname{erfc}\left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}}\right] \end{aligned}$$

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

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

$$c(x, t) =$$

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

where

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

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

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

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

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

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

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

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

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

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

where

$$\begin{aligned} B_3(x,t) = & \frac{v}{(v+u)} \exp \left[\frac{(v-u)x}{2D} \right] \operatorname{erfc} \left[\frac{Rx - ut}{2(DRt)^{1/2}} \right] \\ & + \frac{v}{(v-u)} \exp \left[\frac{(v+u)x}{2D} \right] \operatorname{erfc} \left[\frac{Rx + ut}{2(DRt)^{1/2}} \right] \\ & + \frac{v^2}{2\mu D} \exp \left(\frac{vx}{D} - \frac{\mu t}{R} \right) \operatorname{erfc} \left[\frac{Rx + vt}{2(DRt)^{1/2}} \right] \\ & + \frac{v^2}{2\mu D} \left[\frac{v(2L-x)}{D} + \frac{v^2 t}{DR} + 3 + \frac{v^2}{\mu D} \right] \exp \left(\frac{vL}{D} - \frac{\mu t}{R} \right) \operatorname{erfc} \left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}} \right] \end{aligned}$$

$$\begin{aligned}
& - \frac{v^3}{\mu D} \left(\frac{t}{\pi DR} \right)^{1/2} \exp \left[\frac{vL}{D} - \frac{\mu t}{R} - \frac{R}{4Dt} \left(2L-x + \frac{vt}{R} \right)^2 \right] \\
& + \frac{v(u-v)}{(u+v)^2} \exp \left[\frac{(v+u)x - 2uL}{2D} \right] \operatorname{erfc} \left[\frac{R(2L-x) - ut}{2(DRt)^{1/2}} \right] \\
& - \frac{v(u+v)}{(u-v)^2} \exp \left[\frac{(v-u)x + 2uL}{2D} \right] \operatorname{erfc} \left[\frac{R(2L-x) + ut}{2(DRt)^{1/2}} \right]
\end{aligned}$$

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

and

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

where

$$\begin{aligned}
F_3(x, t) = & \left(\frac{v}{v+w} \right) \exp \left[\frac{(v-w)x}{2D} \right] \operatorname{erfc} \left[\frac{Rx - wt}{2(DRt)^{1/2}} \right] \\
& + \left(\frac{v}{v-w} \right) \exp \left[\frac{(v+w)x}{2D} \right] \operatorname{erfc} \left[\frac{Rx + wt}{2(DRt)^{1/2}} \right] \\
& + \frac{v^2}{2D(\mu-\lambda R)} \exp \left(\frac{vx}{D} - \frac{\mu t}{R} + \lambda t \right) \operatorname{erfc} \left[\frac{Rx + vt}{2(DRt)^{1/2}} \right] \\
& + \frac{v^2}{2D(\mu-\lambda R)} \left[\frac{v(2L-x)}{D} + \frac{v^2 t}{DR} + 3 + \frac{v^2}{D(\mu-\lambda R)} \right] \\
& \exp \left(\frac{vL}{D} - \frac{\mu t}{R} + \lambda t \right) \operatorname{erfc} \left[\frac{R(2L-x) + vt}{2(DRt)^{1/2}} \right] \\
& - \frac{v^3}{D(\mu-\lambda R)} \left(\frac{t}{\pi DR} \right)^{1/2} \exp \left[\frac{vL}{D} - \frac{\mu t}{R} + \lambda t - \frac{R}{4Dt} \left(2L-x + \frac{vt}{R} \right)^2 \right]
\end{aligned}$$

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

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

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

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 ($0 < z \leq 1$).

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_0) 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

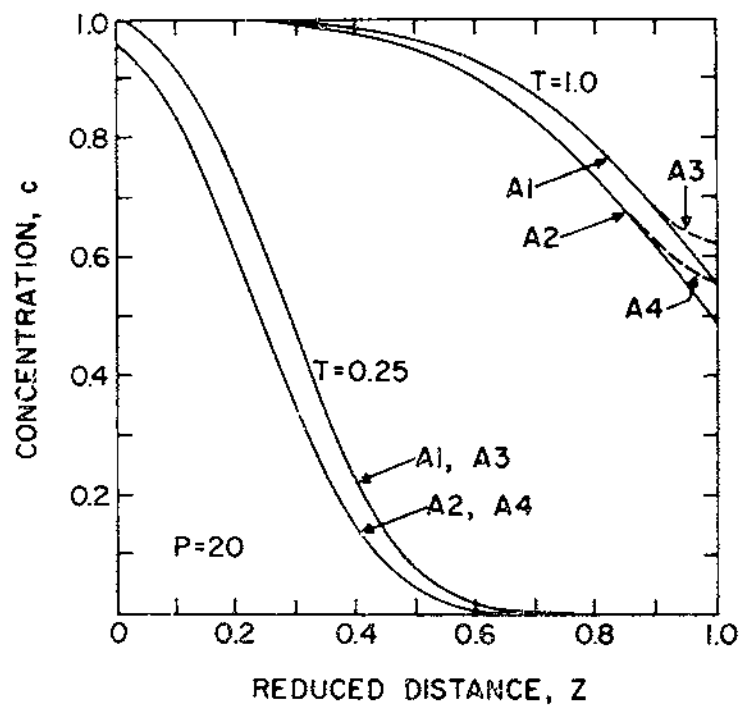
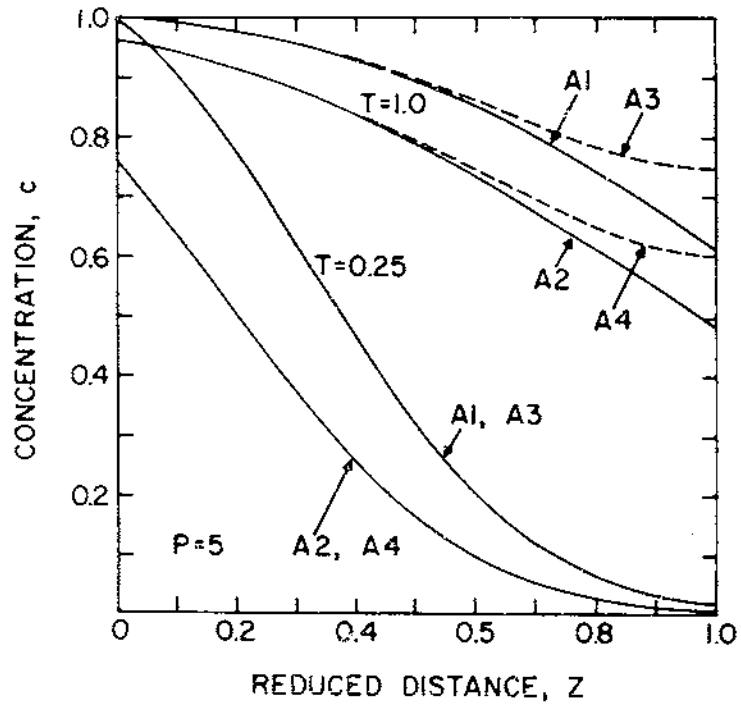


Figure 1. Calculated concentration distributions for $R=1$ and P -values of 5 and 20, respectively. The curves were obtained with the analytical solutions of cases A1, A2, A3, and A4.

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

$$0 < z < .9 - 8/P. \quad [15]$$

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 B 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 conditions 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

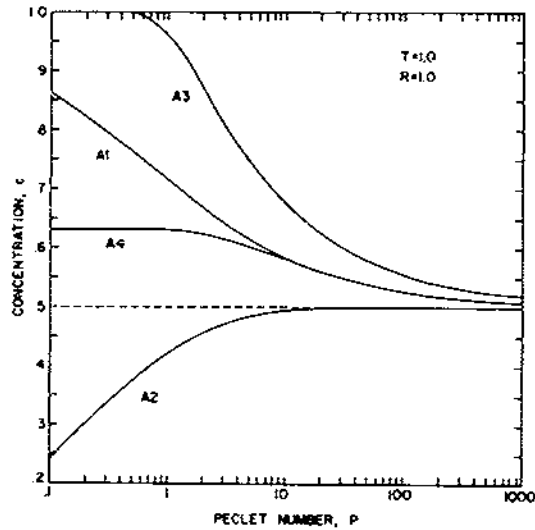


Figure 2. Effect of P on the concentration at $x = L$ and for $T = 1$. The curves were obtained with the analytical solutions of cases A1, A2, A3, and A4.

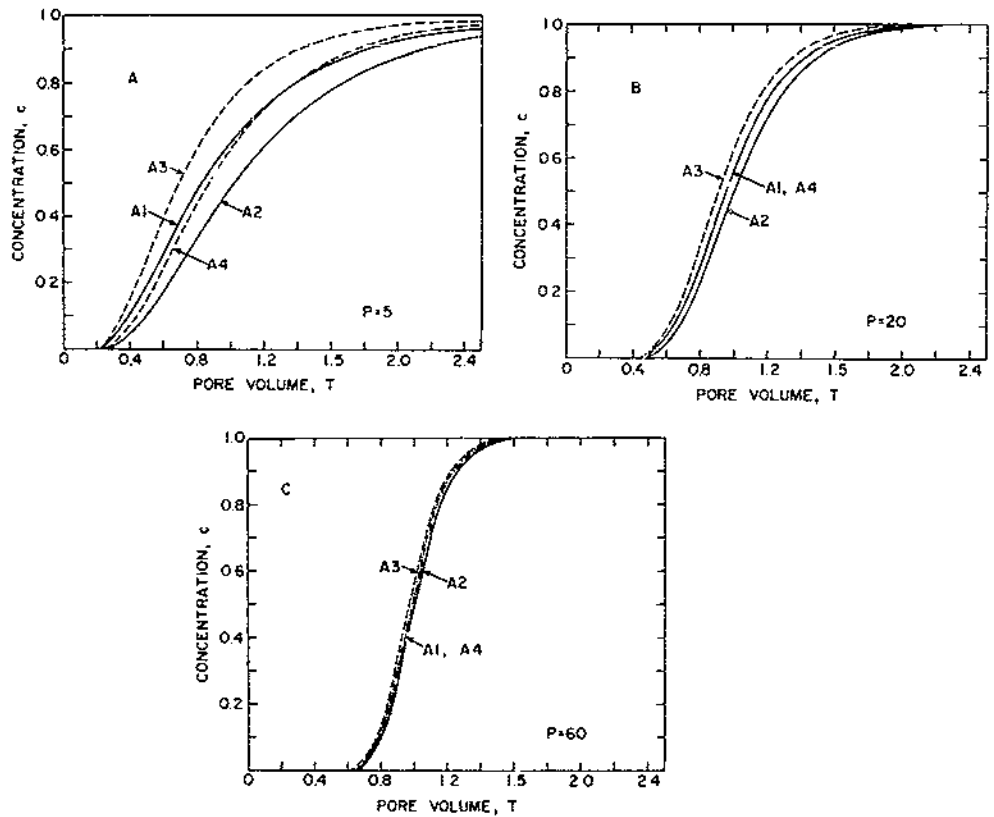


Figure 3. Effect of P on calculated effluent curves for cases A1, A2, A3, and A4.

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

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

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

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

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 $C_0 = 1$ and a value of one for the dimensionless rate term

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

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

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

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

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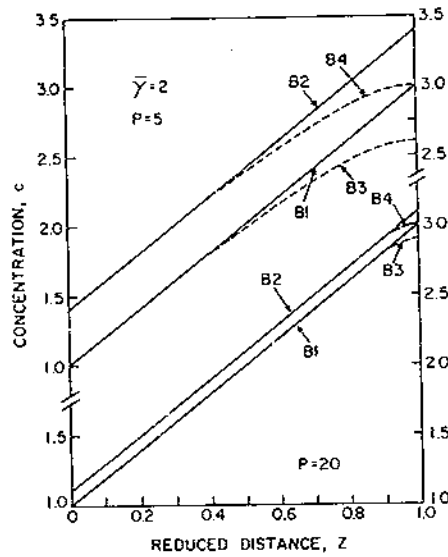


Figure 4. Effect of P on steady-state concentration distributions for cases B1, B2, B3, and B4.

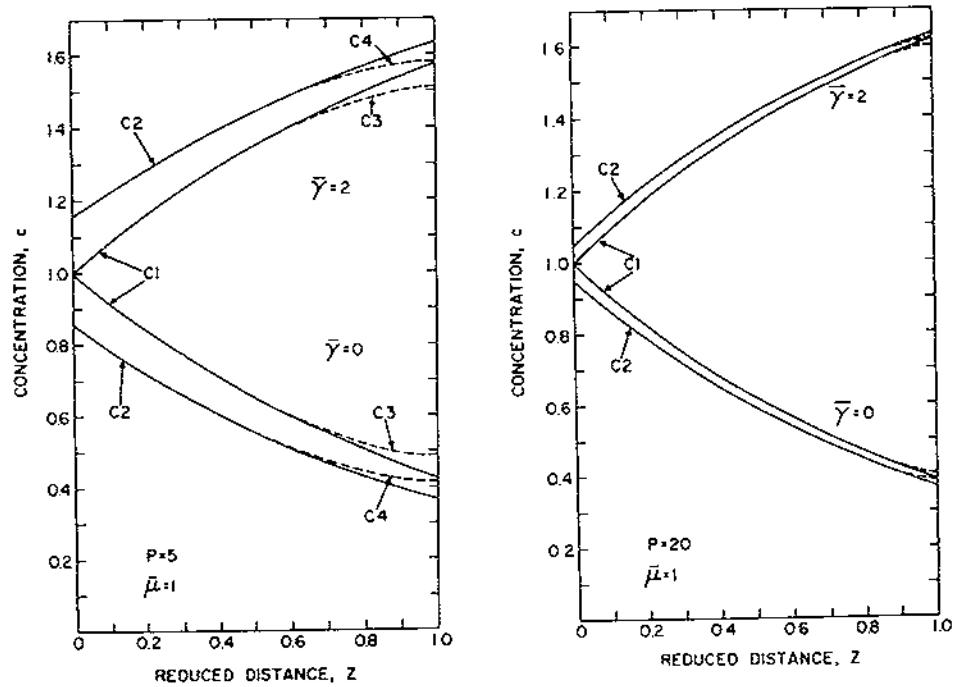


Figure 5. Effect of P on steady-state concentration distributions for cases C1, C2, C3, and C4.

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

| <u>Symbol</u> | <u>Definition</u> |
|--------------------------|---|
| 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:

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

$$B = \operatorname{erfc}\left(\frac{x}{2\sqrt{t}}\right)$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

where

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

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

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

where

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

$$\begin{aligned}
 a_1 &= .2548296 & a_2 &= -.2844967 \\
 a_3 &= 1.421414 & a_4 &= -1.453152 \\
 a_5 &= 1.061405 & &
 \end{aligned}
 \tag{B5}$$

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

$$\text{EXF}(A,B) \approx \frac{1}{\sqrt{\pi}} \exp(A - B^2) / (B + 0.5 / (B + 1. / (B + 1.5 / (B + 2. / (B + 2.5 / (B + 1.))))) \tag{B6}$$

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

$$\text{EXF}(A,B) = 2 \exp(A) - \text{EXF}(A,-B) \tag{B7}$$

The function $\text{EXF}(A,B)$ 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:

$$\begin{aligned}
 |A| > 170 & & |A - B^2| > 170 & \tag{B8} \\
 B < 0 & \text{or} & B > 0 &
 \end{aligned}$$

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 subtraction 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

$$C_{A4} = C_{A2} + G(x,t) \tag{B9}$$

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

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

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

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

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):

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

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

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

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

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 (DELTA) remain constant.

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

| <u>Variable</u> | <u>Definition</u> |
|-----------------|---|
| 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_0 . |
| CA, CB | Constants (C_a, C_b) in several boundary conditions (see table 1). (B14, N1). |
| CI | Constant initial concentration, C_1 . |
| 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 . (E14, N1). |

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

| <u>Variable</u> | <u>Definition</u> |
|-----------------|---|
| EIGEN1(P) | Subroutine to calculate the first 20 eigenvalues (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 eigenvalues (β_i) for the series solution of a finite profile with a third-type boundary condition (C8). |
| EXF(A,B) | Function to calculate $\exp(A) \operatorname{erfc}(B)$. |
| G(I) | Vector containing the first 20 eigenvalues (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

| <u>Variable</u> | <u>Definition</u> |
|-----------------|---|
| P | Column Peclet number: $P = vL/D$. |
| R | Retardation factor. |
| T | Dummy variable for t or $(t-t_0)$. |
| TO | Duration of tracer pulse added to profile, t_0 . |
| 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 | 12345678901234567890123456789012345678901234567890123456789012345678901234567890 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---------|-----------------|--|--------------------|------|------|--------|------|--------|--------|-------|
| A1 | 1 | 2 | | | | | | | | |
| | 2 | | | | | | | | | |
| | 3 | | EXAMPLE A1-1 (P=5) | | | | | | | |
| | 4 | | 1.0 | 4.0 | 1.0 | 1000.0 | .0 | 1.0 | | |
| | 5 | | .0 | 2.0 | 20.0 | 5.0 | 5.0 | 25.0 | | |
| | 6 | | EXAMPLE A1-2 | | | | | | | |
| | 7 | | 25.0 | 37.5 | 3.0 | 5.0 | .0 | 1.0 | | |
| A3 | 1 | 2 | | | | | | | | |
| | 2 | | | | | | | | | |
| | 3 | | EXAMPLE A3-1 (P=5) | | | | | | | |
| | 4 | | 1.0 | 4.0 | 1.0 | 1000.0 | .0 | 1.0 | .0001 | |
| | 5 | | .0 | 2.0 | 20.0 | 20.0 | 5.0 | 5.0 | 25.0 | |
| | 6 | | EXAMPLE A3-2 | | | | | | | |
| | 7 | | 25.0 | 37.5 | 3.0 | 5.0 | .0 | 1.0 | .0001 | |
| B14 | 1 | 1 | | | | | | | | |
| | 2 | | | | | | | | | |
| | 3 | | EXAMPLE B14-1 | | | | | | | |
| | 4 | | 25.0 | 37.5 | 3.0 | .5 | .25 | .0 | .0 | 10.0 |
| C8 | 1 | 2 | | | | | | | | |
| | 2 | | | | | | | | | |
| | 3 | | EXAMPLE C8-1 (P=5) | | | | | | | |
| | 4 | | 1.0 | 4.0 | 1.0 | 1000.0 | .5 | .25 | .0 | 1.0 |
| | 5 | | .0 | 2.0 | 20.0 | 20.0 | 5.0 | 5.0 | 25.0 | .0001 |
| | 6 | | EXAMPLE C8-2 | | | | | | | |
| | 7 | | 25.0 | 37.5 | 3.0 | 5.0 | 5.0 | .25 | .0 | 1.0 |
| N1 | 1 | 2 | | | | | | | | |
| | 2 | | | | | | | | | |
| | 3 | | EXAMPLE A3-1 (P=5) | | | | | | | |
| | 4 | 40 | 125 | 1 | -1 | .5 | .2 | 5.0 | .0 | .0 |
| | 5 | | 1.0 | 4.0 | 1.0 | .0 | 1.0 | .0 | 1000.0 | |
| | 6 | | EXAMPLE B14-1 | | | | | | | |
| | 7 | 40 | 125 | 3 | -1 | 2.5 | .1 | 2.5 | .5 | .0 |
| | | 25.0 | 37.5 | 3.0 | .0 | .0 | 10.0 | 1000.0 | .25 | |

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

EXF

```

FUNCTION 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 CONVECTIVE-DISPERSIVE EQUATION           A1 *
C *
C *       SEMI-INFINITE PROFILE                                     *
C *
C *       NO PRODUCTION OR DECAY                                   *
C *       LINEAR ADSORPTION (R)                                   *
C *       CONSTANT INITIAL CONCENTRATION (CI)                     *
C *       INPUT CONCENTRATION   = C0 (T.LE.TO)                     *
C *                               = 0 (T.GT.TO)                     *
C *
C *****
C
C   IMPLICIT REAL*8 (A-H,C-Z)
C   DIMENSION TITLE(20)
C
C   ----- READ NUMBER OF CURVES TO BE CALCULATED -----
C   READ(5,1000) NC
C   DO 4 K=1,NC
C   READ(5,1001) TITLE
C   WRITE(6,1002) TITLE
C
C   ----- READ AND WRITE INPUT PARAMETERS -----
C   READ(5,1003) V,D,R,TO,CI,C0
C   READ(5,1003) XI,DX,XM,TI,DT,TM
C   WRITE(6,1004) V,D,R,TC,CI,C0
C
C   -----
C   D=D/R
C   V=V/R
C   IF(DX.EQ.0.) DX=1.0
C   IF(DT.EQ.0.) DT=1.0
C   IMAX=(XM+DX-XI)/DX
C   JMAX=(TM+DT-TI)/DT
C   E=0.0
C   DO 4 J=1,JMAX
C   IF(IMAX.GE.J) WRITE(6,1005)
C   TIME=TI+(J-1)*DT
C   DO 4 I=1,IMAX
C   X=XI+(I-1)*DX
C   VVD=0.0
C   IF(X.EQ.0.) GO TO 1
C   VVC=V*R*TIME/X
C 1 DO 2 M=1,2
C   A1=0.0

```

MAIN

```

A2=0.0
T=TIME+(1-M)*T0
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(.2183099*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,CONC1,CONC2

```

C
C

```

1000 FORMAT(I5)
1001 FCRMAT(20A4)
1002 FCRMAT(1H1,10X,82(1H*)/11X,1H*,80X,1H*/11X,1H*,9X,'ONE-DIMENSIONAL
1 CONVECTIVE-DISPERISVE 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.TC)',37X,1H*/11X,1H*,29X,'= 0 (T.GT.TC)'
6,37X,1H*/11X,1H*,80X,1H*/11X,1H*,20A4,1H*/11X,1H*,80X,1H*/11X,82(1
7H*))
1003 FCRMAT(8F10.0)
1004 FCRMAT(//11X,'INPUT PARAMETERS'/11X,16(1H=)//11X,'V =',F12.4,15X,'
1D =',F12.4/11X,'R =',F12.4,15X,'T0 =',F11.4/11X,'CI =',F11.4,15X,'
2CO =',F11.4)
1005 FORMAT(//11X,'DISTANCE',11X,'TIME',7X,'PURE 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 (C1)
*       INPUT CONCENTRATION = C0 (T.LE.T0)
*                           = 0 (T.GT.T0)
*
*       EXAMPLE A1-1 (P=5)
*
*****

```

INPUT PARAMETERS
=====

```

V =      1.0000      D =      4.0000
R =      1.0000      T0 =    1000.0000
C1 =      0.0        C0 =      1.0000

```

| DISTANCE (X) | TIME (T) | PORE VOLUME (VVO) | CONCENTRATION | |
|-----------------|-------------|----------------------|---------------|---------------|
| | | | FIRST-TYPE BC | 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 | 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 | 0.4461 | 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 | 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 (VVC) | CONCENTRATION | |
|-----------------|-------------|----------------------|---------------|---------------|
| | | | FIRST-TYPE BC | 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 (VVC) | CONCENTRATION | |
|-----------------|-------------|----------------------|---------------|---------------|
| | | | FIRST-TYPE BC | 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 | 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 | 0.7602 | 0.7684 |
| 100.0000 | 15.0000 | 3.7500 | 0.7509 | 0.7552 |
| 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-DIMENSIONAL CONVECTIVE DISPERSIVE EQUATION      A3 *
C *
C *      FIRST-TYPE BOUNDARY CONDITION                          *
C *      FINITE PROFILE                                        *
C *
C *      NO PRODUCTION OR DECAY                                *
C *      LINEAR ADSORPTION (R)                                *
C *      CONSTANT INITIAL CONCENTRATION (CI)                  *
C *      INPUT CONCENTRATION  = CO (T.LE.TO)                   *
C *                      = 0 (T.GT.TO)                         *
C *
C *****
C
C
C      IMPLICIT REAL*8 (A-H,C-Z)
C      COMMON G(20)
C      DIMENSION TITLE(20)
C
C      ----- READ NUMBER OF CURVES TO BE GENERATED -----
C      READ(5,1000) NC
C      DO 4 K=1,NC
C      READ(5,1001) TITLE
C      WRITE(6,1002) TITLE
C
C      ----- READ AND WRITE INPUT PARAMETERS -----
C      READ(5,1003) V,D,R,TO,CI,CO,TOL
C      READ(5,1003) XI,DX,XM,XL,TI,DT,TM
C      WRITE(6,1004) V,D,R,TO,CI,CO,XL,TOL
C
C
C      -----
C      D=D/R
C      V=V/R
C      IF(DX.EQ.0.) DX=1.0
C      IF(DT.EQ.0.) DT=1.0
C      XM=DMIN1(XM,XL)
C      P=V*XL/D
C      IMAX=(XM+DX-XI)/DX
C      JMAX=(TM+DT-TI)/DT
C      IF(P.LE.100.) CALL EIGEN1(P)
C      DO 4 J=1,JMAX
C      TIME=TI+(J-1)*DT
C      IF(IMAX.GE.J) WRITE(6,1005)
C      DO 4 I=1,IMAX
C      X=XI+(I-1)*DX

```


MAIN

```

VVD=0.0
IF(X.EQ.0.) GO TO 1
VVD=V*R*TIME/X
1 DO 2 M=1,2
  C=0.0
  T=TIME+(1-M)*TO
  IF(T.LE.C.) 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 CCNDITION',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,'POKE VOLUME',6X,'CONCENTRA
TION',3X,'NUMBER'/14X,'(X)',13X,'(T)',11X,'(VVD)',14X,'(C)',7X,'DF
2 TERMS')
1006 FORMAT(4X,3(5X,F10.4),8X,F10.4,7X,I4)
STOP
END

```

EIGEN1

SUBROUTINE EIGEN1(P)

C
C
C

PURPOSE: TO CALCULATE THE EIGENVALUES

IMPLICIT REAL*8 (A-H,O-Z)

COMMON G(20)

BETA=0.1

DC 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)

PURPOSE: TO CALCULATE CONCENTRATION C

IMPLICIT REAL*8 (A-H,C-Z)
CGMMCN 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

-----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.1.0-10) 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

----- APPROXIMATE SOLUTION -----

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.-E)-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 = C0 (T.LE.T0)
*                          = 0 (T.GT.T0)
*
*       EXAMPLE A3-1   (P=5)
*
*****

```

INPUT PARAMETERS
=====

```

V =      1.0000          D =      4.0000
R =      1.0000          T0 =    1000.0000
CI =     0.0            C0 =      1.0000
XL =    20.0000          TGL =   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 | C.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 | C.8333 | 0.6209 | 6 |
| 8.0000 | 5.0000 | C.6250 | 0.4648 | 6 |
| 10.0000 | 5.0000 | C.5000 | 0.3225 | 6 |
| 12.0000 | 5.0000 | 0.4167 | 0.2064 | 6 |
| 14.0000 | 5.0000 | C.3571 | 0.1216 | 6 |
| 16.0000 | 5.0000 | C.3125 | 0.0661 | 6 |
| 18.0000 | 5.0000 | C.2778 | 0.0348 | 6 |
| 20.0000 | 5.0000 | C.2500 | 0.0240 | 6 |

| DISTANCE (X) | TIME (T) | PORE VOLUME (VVO) | CONCENTRATION (C) | NUMBER OF TERMS |
|-----------------|-------------|----------------------|----------------------|--------------------|
| 0.0 | 10.0000 | C.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 | 0.5530 | 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 | 0.8720 | 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 (VVC) | 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 (VVC) | 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        TBL =     0.000100

```

CALCULATED EIGENVALUES

=====

```

3.050337   6.102126   9.156690   12.215114   15.278191
18.346412  21.419993   24.498930   27.583053   30.672083
33.765670  36.863467   39.965076   43.070143   46.178327
49.289314  52.402819   55.518585   58.636381   61.750003

```

| 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
C IMPLICIT REAL*8 (A-H,C-Z)
C DIMENSION TITLE(20)
C
C ----- READ NUMBER OF CURVES TO BE CALCULATED -----
C READ(5,1000) NC
C DO 4 K=1,NC
C READ(5,1001) TITLE
C WRITE(6,1002) TITLE
C
C ----- READ AND WRITE INPUT PARAMETERS -----
C READ(5,1003) V,D,R,DZERO,DBND,CI,CA,CB
C READ(5,1003) XI,DX,XM,II,DT,TM
C WRITE(6,1004) V,D,R,DZERO,DBND,CI,CA,CB
C
C -----
C D=D/R
C V=V/R
C DZERO=DZERO/R
C S=V**2-4.*DBND*D
C IF(S.LE.0.) GO TO 5
C Y=DSQRT(S)
C IF(DX.EQ.0.) DX=1.0
C IF(DT.EQ.0.) DT=1.0
C IMAX=(XM+DX-XI)/DX
C JMAX=(TM+DT-II)/DT
C DO 4 J=1,JMAX
C T=II+(J-1)*DT
C IF(IMAX.GE.J) WRITE(6,1005)
C DO 4 I=1,IMAX
C X=XI+(I-1)*DX
C VVD=0.0
C IF(X.EQ.0.) GO TO 1

```


MAIN

```

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(0.00,A1/S)
AP=0.5*EXF(P,A2/S)
AZ=DSQRT(.3183099*T/D)*EXF(-(A1/S)**2,0.00)
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=C I+(CA-CI)*A+CB*B+CZERO*(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,VVG,CCNC
GO TO 6
5 WRITE(6,1007)
6 CONTINUE

```

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,'THIRD-TYPE BOUNDARY CCNDITION',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,'PGRE VOLUME',6X,'CONCENTR
1ATION'/14X,'(X)',13X,'(T)',11X,'(VVO)',14X,'(C)'/)
1006 FCRMAT(4X,3(5X,F10.4),8X,F10.4)
1007 FORMAT(///5X/6(1H*),' CBND IS TOO LARGE, THIS CASE NOT EXECJTED ',
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 | 1.7657 | 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 | 4.5309 |
| 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 | 1.2068 |
| 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 | 0.8330 |
| 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 (VVG) | CONCENTRATION (C) |
|-----------------|-------------|----------------------|----------------------|
| 0.0 | 7.5000 | 0.0 | 1.0390 |
| 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 | 5.8818 |
| 45.0000 | 7.5000 | 4.1667 | 6.2657 |
| 50.0000 | 7.5000 | 3.7500 | 6.3404 |
| 55.0000 | 7.5000 | 3.4091 | 6.0505 |
| 60.0000 | 7.5000 | 3.1250 | 5.4071 |
| 65.0000 | 7.5000 | 2.8846 | 4.5184 |
| 70.0000 | 7.5000 | 2.6786 | 3.5865 |
| 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 | 1.9727 | 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-DIMENSIONAL CONVECTIVE DISPERSIVE EQUATION      C8 *
C *
C *      FIRST-TYPE BOUNCARY CONDITION *
C *      FINITE PROFILE *
C *
C *      ZERO-ORDER PRODUCTION (DZERO) *
C *      FIRST-ORDER DECAY (DONE) *
C *      LINEAR ADSORPTION (R) *
C *      CONSTANT INITIAL CONCENTRATION (CI) *
C *      INPUT CONCENTRATION = CO (T.LE.TO) *
C *                          = 0 (T.GT.TO) *
C *
C *****
C
C
C      IMPLICIT REAL*8 (A-H,C-Z)
C      COMMON G(20)
C      DIMENSION TITLE(20)
C
C      ----- READ NUMBER OF CURVES TO BE GENERATED -----
C      READ(5,1000) NC
C      DO 4 K=1,NC
C      READ(5,1001) TITLE
C      WRITE(6,1002) TITLE
C
C      ----- READ AND WRITE INPUT PARAMETERS -----
C      READ(5,1003) V,D,R,TO,CZERO,DONE,CI,CO
C      READ(5,1003) XI,DX,XM,XL,TI,DT,TM,TOL
C      WRITE(6,1004) V,D,R,TC,DZERO,CI,DONE,CO,TUL
C
C      -----
C      D=D/R
C      V=V/R
C      DZERO=DZERO/R
C      DONE=DONE/R
C      DZD=DZERO/DONE
C      IF(DX.EQ.0.) DX=1.0
C      IF(DT.EQ.0.) DT=1.0
C      XM=DMIN1(XM,XL)
C      P=V*XL/D
C      IMAX=(XM+DX-XI)/DX
C      JMAX=(TM+DT-TI)/DT
C      IF(P.LE.100.) CALL EIGEN3(P)
C      DO 4 J=1,JMAX
C      TIME=TI+(J-1)*DT

```

MAIN

```

IF(IMAX.GE.J) WRITE(6,1005)
DC 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(3,V,D,DONE,X,TIME,XL,TOL,N,1)
CCNC=DZD+(CI-DZD)*A+(CO-DZD)*B
T=TIME-TO
IF(T.LE.0.) GO TO 2
CALL CCNS(3,V,D,DONE,X,T,XL,TOL,N,1)
CONC=CCNC-CO*B
2 CONTINUE
4 WRITE(6,1006) X,TIME,VVC,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*,00X,1H*/11X,1H*,9
2X,'THIRD-TYPE BOUNDARY CCNDITION',42X,1H*/11X,1H*,9X,'FINITE PROFI
3LE',57X,1H*/11X,1H*,80X,1H*/11X,1H*,9X,'ZERO-ORDER PRCDUCTION (DZE
4RC)',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
6CNCENTRATION (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,'TCL =',F10.5
3)
1005 FORMAT(//11X,'DISTANCE',11X,'TIME',7X,'PORE VOLUME',6X,'CONCENTRA
TION',3X,'NUMBER'/14X,'(X)',13X,'(T)',11X,'(VVO)',14X,'(C)',7X,'OF
2 TERMS')
1006 FORMAT(4X,3(5X,F10.4),6X,F10.4,7X,I4,F10.4)
STOP
END

```

EIGEN3

SUBROUTINE EIGEN3(P)

PURPOSE: TO CALCULATE THE EIGENVALUES

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

CCNS

C SUBROUTINE CONS(C,V,D,DCNE,X,T,XL,TOL,I,M)

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.*DCNE*C/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.).GR.((P-40.*V*T/XL).GT.5.)) GO TO 4

EX=0.5*Q-0.25*V*V*T/D-DCNE*T

C -----SERIES SOLUTION-----

C=0.0

DO 2 J=1,10

LC=0.0

DO 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+DCNE*XL**2/D))

1 DC=DC+TERM

C=C+DC

IF(DABS(DC/C).LT.TOL) GO TO 3

2 CONTINUE

3 IF(M.EQ.0) RETURN

C=2.*V*(EXP(.5*(Q-QU),E)+LV*EXP(.5*(Q+QU)-PU,E))/((U+V)*(1.-UV**2*
1EXP(-PU,E)))-C

RETURN

C ----- APPROXIMATE SOLUTION -----

4 S=DSQRT(4.*D*T)

UX=2.*XL-X

AM=(V-V*T)/S

AP=(V+V*T)/S

BM=(UX-V*T)/S

CCNS

```

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-L)*EXF(DP,FP)+0.5*V**2/(DONE*D)*EXF(Q-DONE*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))*EXF(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*((1.-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-DISPERIVE EQUATION
*
*       THIRD-TYPE BOUNDARY CONDITION
*       FINITE PROFILE
*
*       ZERO-ORDER PRODUCTION (DZERO)
*       FIRST-ORDER DECAY (DGNE)
*       LINEAR ADSORPTION (R)
*       CONSTANT INITIAL CONCENTRATION (CI)
*       INPUT CCNTRATION = 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
DGNE =   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 (VVG) | 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 | 1.4554 | 6 |
| 8.0000 | 5.0000 | 0.6250 | 1.4570 | 6 |
| 10.0000 | 5.0000 | 0.5000 | 1.4518 | 6 |
| 12.0000 | 5.0000 | 0.4167 | 1.4441 | 6 |
| 14.0000 | 5.0000 | 0.3571 | 1.4374 | 6 |
| 16.0000 | 5.0000 | 0.3125 | 1.4327 | 6 |
| 18.0000 | 5.0000 | 0.2778 | 1.4299 | 6 |
| 20.0000 | 5.0000 | 0.2500 | 1.4250 | 6 |

| DISTANCE (X) | TIME (T) | PORE VOLUME (VVG) | 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 (VVC) | 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 CCNDITICN
*       FINITE PROFILE
*
*       ZERO-ORDER PRODUCTION (DZERC)
*       FIRST-ORDER DECAY (DCNE)
*       LINEAR ADSORPTION (K)
*       CONSTANT INITIAL CONCENTRATION (CI)
*       INPUT CONCENTRATION = CO (I.LE.TO)
*                           = 0 (T.GT.TO)
*
*       EXAMPLE C8-2
*
*****

```

INPUT PARAMETERS
=====

```

V =      25.0000          D =      37.5000
R =       3.0000          TO =       5.0000
DZERC =   0.5000          CI =        0.0
DCNE =    0.2500          CO =      1.00000
TOL =    0.00010

```

CALCULATED EIGENVALUES
=====

```

 2.964207   5.931010   8.902794   11.881558   14.868811
17.865546  20.872271  23.889065  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) | PGRE VCLUME (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 (VVG) | 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 (VVG) | 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 | 4.8777 | 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 CONVECTIVE-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 BOUNDARY CONDITION (DBND)
C *
C *****
C
C
C      DIMENSION TITLE(20),C(200),F(200),U(200),X(200)
C
C      -----
C      READ(5,1000) NC
C      DO 14 KK=1,NC
C      READ(5,1001) TITLE
C      WRITE(6,1002) TITLE
C
C      ----- READ AND WRITE INPUT PARAMETERS -----
C      READ(5,1003) NE,NSTEPS,KSURF,KINIT,DELX,DELTA,PRDEL,DZERO,DONE,DBND
C      READ(5,1004) V,D,R,CI,CA,CB,TO
C      IF(KSURF.EQ.3) WRITE(6,1005)
C      IF(KSURF.EQ.1) WRITE(6,1006)
C      WRITE(6,1007)
C      DB=ABS(DBND)
C      IF(DB.LT.0.00001) CB=0
C      WRITE(6,1008) NE,DELTA,TO,NSTEPS,DELX,DZERO,V,CI,DONE,D,CA,DBND,R,C
C      18
C
C      -----
C      NN=NE+1
C      IF(KINIT) 1,3,5
C      1 DO 2 I=1,NN
C      2 C(I)=CI
C      GO TO 6
C      3 Y=SQRT(V*V+4.*DONE*D)
C      DO 4 I=1,NN
C      4 C(I)=DZERO/DONE+(C I-DZERO/DONE)*EXP((V-Y)*X(I)/(2.*D))
C      GO TO 6
C      5 READ(5,1004) (C(I),I=1,NN)
C      6 DO 7 I=1,NN
C      7 X(I)=(I-1)*DELX

```

MAIN

```

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) J(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)+E0*C(2)+0.5*DZERO+V*(CA+BND*EXT)
```

```
DO 8 I=2,NE
```

```
8 F(I)=BO*C(I-1)+D2*C(I)+E0*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
```

MAIN

```

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 (DLNE)',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-DISPERISVE EQUATION
*
*   NUMERICAL SOLUTION
*
*   LINEAR EQUILIBRIUM ADSORPTION (R)
*   ZERO-ORDER PRODUCTION (DZERO)
*   FIRST-ORDER DECAY (DCNE)
*   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          LZERO =    0.0
V =         1.0000          CI =     0.0          DJNE =    0.0
D =         4.0000          CA =    1.0000          JBND =    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  0.5818    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  0.7750    4.50  0.7372
5.00  0.6595    5.50  0.6610    6.00  0.6219    6.50  0.5826    7.00  0.5455
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 0.1050
15.00 0.0909    15.50 0.0779    16.00 0.0666    16.50 0.0567    17.00 0.0485
17.50 0.0413    18.00 0.0357    18.50 0.0313    19.00 0.0265    19.50 0.0200
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 | 0.9855 | 1.50 | 0.9733 | 2.00 | 0.9628 |
| 2.50 | 0.9506 | 3.00 | 0.9379 | 3.50 | 0.9257 | 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 | 0.9657 | 3.50 | 0.9628 | 4.00 | 0.9533 | 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 | 0.8653 | 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 | 0.9985 | 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 | 0.9625 | 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 (K)
*      ZERO-ORDER PRODUCTION (DZERC)
*      FIRST-ORDER DECAY (DONE)
*      DECAYING BOUNDARY CONDITION (DBND)
*
*      EXAMPLE B14-1
*
*      THIRD-TYPE BOUNDARY CONDITION
*
*****

```

INPUT PARAMETERS
=====

```

NE =      40          DELT = 0.1000          TO = 1000.0000
NSTEPS = 125         DELX = 2.5000          JZERO = 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

```

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 | | | | | | | | |

CONCENTRATION AT TIME = 2.5000

| DEPTH | VALUE | DEPTH | VALUE | DEPTH | VALUE | DEPTH | VALUE | DEPTH | VALUE |
|--------|--------|-------|--------|-------|--------|-------|--------|-------|--------|
| 0.0 | 5.6314 | 2.50 | 6.0518 | 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 | | | | | | | | |

CONCENTRATION AT TIME = 5.0000

| DEPTH | VALUE | DEPTH | VALUE | DEPTH | VALUE | DEPTH | VALUE | DEPTH | VALUE |
|--------|--------|-------|--------|-------|--------|-------|--------|-------|--------|
| 0.0 | 3.0357 | 2.50 | 3.3212 | 5.00 | 3.6457 | 7.50 | 3.9792 | 10.00 | 4.3305 |
| 12.50 | 4.6959 | 15.00 | 5.0667 | 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 | 6.3767 | 35.00 | 6.1158 |
| 37.50 | 5.7144 | 40.00 | 5.1572 | 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 | 0.5795 | 67.50 | 0.9127 | 70.00 | 0.8740 | 72.50 | 0.8529 |
| 75.00 | 0.8422 | 77.50 | 0.8371 | 80.00 | 0.8346 | 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 | | | | | | | | |

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 | 6.3303 |
| 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 | 1.2698 |
| 100.00 | 1.2898 | | | | | | | | |

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 | 2.2266 |
| 25.00 | 2.4214 | 27.50 | 2.6255 | 30.00 | 2.8415 | 32.50 | 3.0700 | 35.00 | 3.3112 |
| 37.50 | 3.5551 | 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 | 6.3035 | 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 | | | | | | | | |

CONCENTRATION AT TIME = 12.5000

| DEPTH | VALUE | DEPTH | VALUE | DEPTH | VALUE | DEPTH | VALUE | DEPTH | VALUE |
|--------|--------|-------|--------|-------|--------|-------|--------|-------|--------|
| 0.0 | 0.4910 | 2.50 | 0.5767 | 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 | | | | | | | | |

END