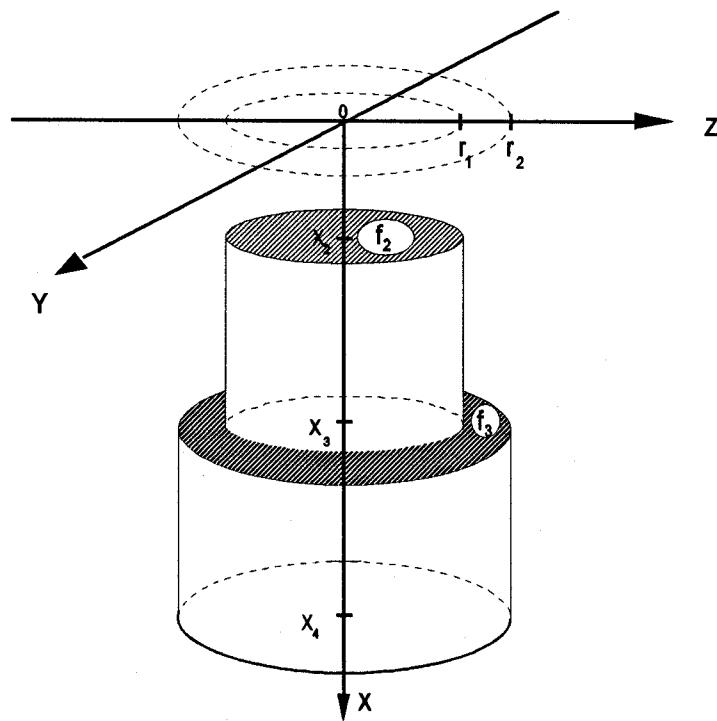


N3DADE: A COMPUTER PROGRAM FOR EVALUATING NONEQUILIBRIUM THREE-DIMENSIONAL SOLUTE TRANSPORT IN POROUS MEDIA



Research Report No. 143

September 1997

U. S. SALINITY LABORATORY
AGRICULTURAL RESEARCH SERVICE
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**N3DADE: A COMPUTER PROGRAM FOR EVALUATING
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DISCLAIMER

The N3DADE code was developed primarily for research purposes to evaluate analytical solutions for nonequilibrium transport in three-dimensional porous media as reported by *Leij et al.* [1993]. Although the program has been verified for several transport scenarios and using a variety of transport parameters, no guarantee can be given that the program is completely error-free, or functions according to the intent of all users. Computational efficiency and user-friendliness were not of major concern during code development. The N3DADE computer program is a public domain code, which may be used and copied freely. Users are encouraged to communicate their experiences with N3DADE to the authors at the following address

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ACKNOWLEDGMENTS

The authors wish to thank Walter Russell for preparing the illustrations and Rien van Genuchten for his careful review of this report.

ABSTRACT

This research report documents the Fortran program N3DADE (Nonequilibrium 3-Dimensional Advection-Dispersion Equation) which may be used to evaluate analytical solutions described by *Leij et al.* [1993]. The analytical solutions pertain to selected cases of three-dimensional solute transport during steady unidirectional water flow in porous media of semi-infinite length in the longitudinal direction, and of infinite length in the transverse directions. The solutions may also be applied to one- and two-dimensional problems. Transport and flow properties of the medium are assumed to be macroscopically uniform. Nonequilibrium solute transfer can occur between two domains in either the liquid or the adsorbed phase. The transport equation contains terms for solute movement by advection and dispersion, and for solute retardation, first-order decay, and zero-order production. Solute concentrations are calculated as a function of time and space in a three-dimensional Cartesian coordinate system.

This report serves as both a user manual for the program and as documentation of the general analytical solutions of the boundary, initial and production value problems involved. A comprehensive set of specific solutions is presented using Dirac, Heaviside and exponential functions to describe the initial, boundary and production profiles. A rectangular or circular inflow area is specified for the boundary value problem, while for the initial and production value problems the respective initial and production profiles are defined for parallelepipedal, cylindrical, or spherical regions of the soil. Solutions are given for volume-averaged or resident concentrations, as well as for flux-averaged or flowing concentrations. The report also provides a list of main program variables, the format of the input file, listings of sample input and output files, and the source code N3DADE.FOR.

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LIST OF SYMBOLS

<i>Symbol</i>	<i>Description</i>
a_0	constant defined by (36a)
a_1	constant defined by (22a)
a_2	constant defined by (36b)
b	constant defined by (22b)
C_k	solute concentrations of phase k ($k=1,2$) (Table 1)
d	constant defined by (36c)
f	fraction of equilibrium or mobile sorption sites (Table 1)
f_i	value of initial concentration ($i=1,2,\dots,e$)
$f(X,Y,Z)$	initial concentration profile ($=f_X(X)f_Y(Y)f_Z(Z)$)
g_i	value of input concentration ($i=1,2,\dots,e$)
$g(Y,Z,T)$	input function ($=g_Y(Y)g_Z(Z)g_T(T)$)
G	auxiliary longitudinal function (Table 2)
$h(X,T)$	auxiliary equilibrium dummy function (37)
$H_n(\tau;T)$	auxiliary nonequilibrium function ($n=0,1$) (46)
I_0, I_1	modified Bessel function of orders zero and one
J	Goldstein's J -function (61)
p	variable in Goldstein's J -function (60a, 62a)
P_x, P_y, P_z	Peclet number (Table 1)
q	variable in Goldstein's J -function (60b, 62b)
r	variable for Laplace transformation with respect to X (25)
r_{\pm}	roots of Laplace variable r (31)
r_c	circular coordinate (78)
r_s	spherical coordinate (79)
R	retardation factor (Table 1)
s	variable for Laplace transformation with respect to T (14)
s^*	modified Laplace variable (37)
T	time (Table 1)
X	longitudinal position (Table 1)
Y	transversal position (Table 1)
Z	transversal position (Table 1)
w	constant in exponential profile for BVP (89b)
 <i>Greek</i>	
α	first-order kinetic rate coefficient (3), constant in exponential profile (30)
β	partition coefficient (Table 1)
Γ	auxiliary transverse functions (Table 3)
η	dummy variable for integration with respect to time
κ	variable for Fourier transformation with respect to Z (29)
γ	variable for Fourier transformation with respect to Y (29)
λ_k	value of zero-order production factor ($i=1,2,\dots,e$ and $k=1,2$)

$\lambda_k(X,Y,Z)$	production profile ($=\lambda_{kx}(X)\lambda_{ky}(Y)\lambda_{kz}(Z)$)
μ_k	first-order decay coefficients in phase k ($k=1,2$) (Table 1)
ξ	dummy variable for integration with respect to X
τ	dummy variable for integration with respect to time
Ω	dummy variable for integration with respect to Z (43)
φ	dummy variable for integration with respect to Y (43)
ω	mass transfer coefficient (Table 1)

Subscripts

F	flux-averaged concentration mode
R	resident concentration mode
T	total concentration mode (12)
1	equilibrium (Table 1)
2	nonequilibrium (Table 1)

Superscripts

B	boundary value problem (BVP)
I	initial value problem (IVP)
P	production value problem (PVP)

Miscellaneous

\mathcal{L}	Laplace transformation
\mathcal{F}	Fourier transformation
$-$	Laplace transformation with respect to T (14)
\sim	Laplace transformation with respect to X (25)
\wedge	Fourier transformation with respect to Y and Z (29)

1. INTRODUCTION

The N3DADE code evaluates analytical solutions published by *Leij et al.* [1993] for nonequilibrium solute transport in three-dimensional porous media (semi-infinite in the longitudinal direction and infinite in the transversal directions) during steady unidirectional flow. The code is an extension of the program 3DADE, which considers a number of three-dimensional solutions for equilibrium transport [*Leij and Bradford*, 1994]. By selecting appropriate nonequilibrium parameters, the solutions in N3DADE may provide similar results as those in 3DADE. However, computational errors will likely arise if the parameters in N3DADE are selected such that the resulting problem becomes an equilibrium application. We further note that N3DADE has more options for specifying mathematical conditions than 3DADE.

Analytical modeling of transport problems may increasingly seem less attractive since many transport problems are nonlinear, whereas advances in software and hardware have made it quite convenient to use numerical models. Analytical solutions, however, can still be useful for such applications as: (i) assessing the performance of numerical solution techniques, (ii) gaining a better understanding of the importance of different transport parameters, (iii) estimating model parameters with inverse methods, and (iv) predicting the fate and movement of solutes for large temporal or spatial scales or if there is no detailed knowledge of the input parameters.

Bimodal nonequilibrium models have been frequently used for one-dimensional solute transport [cf. *van Genuchten and Wierenga*, 1977; *Nkedi-Kizza et al.*, 1983]. Such models simplify the description of nonequilibrium processes by assuming that either the liquid phase consists of a "mobile" and an "immobile" region [*van Genuchten and Wierenga*, 1976] or that the adsorbed phase contains sites with "instantaneous" and "kinetic" sorption [*Selim et al.*, 1976]. *Nkedi-Kizza et al.* [1984] showed that these respective "physical" and "chemical" nonequilibrium models can be described with the same equation if appropriate dimensionless variables are being introduced. The physical and chemical nonequilibrium models can be extended to include both types of nonequilibrium simultaneously [*Brusseau et al.*, 1989]. Analytical solutions for one-dimensional physical and chemical nonequilibrium models have been provided in the soil science and hydrology literature by *van Genuchten and Wierenga* [1976], *Lassey* [1988], and *van Genuchten and Wagenet* [1989],

among others, while nonequilibrium models have long been used in chemical and petroleum engineering [*Klinkenberg*, 1948; *Hester and Vermeulen*, 1952; *Coats and Smith*, 1964; *Villermaux and van Swaay*, 1969]. In spite of the fact that many transport problems are actually multidimensional, relatively few analytical solutions have been reported for two- and three-dimensional nonequilibrium transport [cf. *Goltz and Roberts*, 1986].

The purpose of this report is to provide a convenient way to evaluate the fairly lengthy and somewhat cumbersome analytical solutions reported by *Leij et al.* [1993]. Chapter 2 presents the mathematical statement of the problem, including the definition of model parameters and the formulation of the governing equation and the auxiliary conditions. Solution are derived for general input, initial, and production profiles. In Chapter 3 we define specific input, initial, and production profiles using Dirac, Heaviside, and exponential functions for rectangular, circular, or spherical regions, and we subsequently formulate analytical solutions for these conditions. A Fortran program used to evaluate the analytical solutions is described in Chapter 4. A detailed outline of the input file is also provided in Appendix B. Examples of predictions obtained with the program are given in Chapter 5. The Appendices contain supplementary material such as the major program variables, listings of the input and output files for the examples discussed in Chapter 5, as well as a listing of the source code.

It is not necessary to read the entire report prior to using the program. However, we recommend to first examine the governing equations and the definition of transport parameters in Chapter 2, as well as the explanation of the input, initial, and production profiles in Chapter 3; this should provide users a clearer picture of what type of problem can be modeled. Furthermore, it is necessary to consult Appendix B for preparing the input file. Run-time errors or erratic results may be encountered because of possible instabilities during evaluation of integrals or special functions, or if the use of an equilibrium model would be more appropriate. In such an event, the user may want to study the solutions in the report more closely to determine if the program can be expected to handle the specified conditions or the imposed parameter values.

2. GENERAL SOLUTIONS

The concepts of chemical and physical nonequilibrium are outlined in this chapter by presenting the corresponding dimensional transport models, and defining all model parameters. The two types of models are transformed to the same dimensionless bimodal nonequilibrium model, which is subsequently used for all further analysis. The governing equations are solved for general boundary, initial, and production conditions using a sequence of Laplace and Fourier transforms. Solutions of the boundary, initial, and production value problems will be provided.

2.1. Problem Statement

Solute movement is studied analytically by making the admittedly restrictive assumption that the porous medium is isotropic and that there is one-dimensional steady flow — both the pore-water velocity and the dispersion coefficients are then constant with respect to time and space. Solutes may be subject to linear retardation (i.e., equilibrium adsorption is described with a linear isotherm), and zero- and first-order production or degradation. Nonequilibrium is attributed to differences in adsorption sites, or to the presence of mobile and immobile fluid regions.

In the two-site model, nonequilibrium sorption for type-2 sites is typically described with a first-order rate law while equilibrium sorption is assumed for type-1 sites [Selim *et al.*, 1976; Cameron and Khute, 1977]. The governing equations for this "chemical" nonequilibrium model may be written as

$$\left(1 + \frac{f\rho k}{\theta}\right) \frac{\partial c}{\partial t} = D_x \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} + D_y \frac{\partial^2 c}{\partial y^2} + D_z \frac{\partial^2 c}{\partial z^2} - \frac{\alpha \rho}{\theta} [(1-f)kc - s_k] - \mu_l c - \frac{f\rho k \mu_{s,e}}{\theta} c + \lambda_l(x,y,z) + \frac{f\rho \lambda_{s,e}(x,y,z)}{\theta} \quad (1)$$

$$\frac{\partial s_k}{\partial t} = \alpha [(1-f)kc - s_k] - \mu_{s,k} s_k + (1-f)\lambda_{s,k}(x,y,z) \quad (2)$$

where c is the resident solute concentration in the liquid phase (ML^{-3}), s_k is the concentration in the adsorbed phase for type-2 sites (MM^{-1}); t is time (T); x is the position (L) in the direction of flow; y and z are rectangular coordinates perpendicular to the flow direction (L); D_x is a longitudinal

dispersion coefficient (L^2T^{-1}) for the x direction; D_y and D_z are transverse dispersion coefficients for the y and z directions, respectively; θ is the volumetric water content (L^3L^{-3}); v is the macroscopically averaged pore-water velocity (LT^{-1}); f is the fraction of type-1 exchange sites, ρ is the bulk density (ML^{-3}); k is a distribution coefficient for linear sorption (ML^{-3}), α is a first-order kinetic rate coefficient (T^{-1}); μ_l and μ_s are first-order decay coefficients for degradation in the liquid and adsorbed phases, respectively (T^{-1}); and $\lambda_{l,m}$ ($ML^{-3}T^{-1}$) and $\lambda_{s,m}$ ($MM^{-1}T^{-1}$) are position dependent zero-order rate coefficients for solute production in the liquid and adsorbed phases, respectively. The subscripts e and k refer to equilibrium and kinetic exchange sites, and l and s denote the liquid and adsorbed phases, respectively.

The "physical" nonequilibrium model assumes that the liquid region can be partitioned into mobile (or flowing) and immobile (or stagnant) regions, that solute movement occurs by advection and dispersion in the mobile region, and that solute exchange between the two regions occurs by first-order diffusion [Coats and Smith, 1964; van Genuchten and Wierenga, 1976]. The governing equations for the two-region model are

$$(\theta_m + f\rho k) \frac{\partial c_m}{\partial t} = \theta D_x \frac{\partial^2 c_m}{\partial x^2} - \theta v \frac{\partial c_m}{\partial x} + \theta D_y \frac{\partial^2 c_m}{\partial y^2} + \theta D_z \frac{\partial^2 c_m}{\partial z^2} - \alpha(c_m - c_{im}) - (\theta_m \mu_{l,m} + f\rho k \mu_{s,m}) c_m + \theta_m \lambda_{l,m}(x, y, z) + f\rho \lambda_{s,m}(x, y, z) \quad (3)$$

$$[\theta_{im} + (1-f)\rho k] \frac{\partial c_{im}}{\partial t} = \alpha(c_m - c_{im}) - [\theta_{im} \mu_{l,im} + (1-f)\rho k \mu_{s,im}] c_{im} + \theta_{im} \lambda_{l,im}(x, y, z) + (1-f)\rho \lambda_{s,im}(x, y, z) \quad (4)$$

where in this case f represents the fraction of sorption sites in equilibrium with the fluid of the mobile region and α is a first-order mass transfer coefficient (T^{-1}); the subscripts m and im refer to the mobile and immobile liquid regions, respectively, and where $\theta = \theta_m + \theta_{im}$.

The two-site and the two-region models can be cast in the same dimensionless form using the parameters listed in Table 1. Notice that several parameters in Table 1 are expressed in terms of an arbitrary characteristic concentration, c_o , and characteristic length, L . The following dimensionless model is obtained in this way:

$$\beta R \frac{\partial C_1}{\partial T} = \frac{1}{P_X} \frac{\partial^2 C_1}{\partial X^2} - \frac{\partial C_1}{\partial X} + \frac{1}{P_Y} \frac{\partial^2 C_1}{\partial Y^2} + \frac{1}{P_Z} \frac{\partial^2 C_1}{\partial Z^2} + \omega(C_2 - C_1) - \mu_1 C_1 + \lambda_1(X, Y, Z) \quad (5)$$

$$(1 - \beta)R \frac{\partial C_2}{\partial T} = \omega(C_1 - C_2) - \mu_2 C_2 + \lambda_2(X, Y, Z) \quad (6)$$

where β is a partition coefficient; R is a retardation factor; C_1 and C_2 are equilibrium and nonequilibrium resident concentrations, respectively; T is time; X is the longitudinal coordinate; Y and Z are transverse coordinates; P_X , P_Y , and P_Z are the Peclet numbers in the X , Y , and Z directions; ω is a mass transfer coefficient; μ and λ are dimensionless first-order decay and zero-order production terms; and the subscripts 1 and 2 refer to the equilibrium and nonequilibrium phases, respectively. The magnitude of several dimensionless parameters depends also on the arbitrary constants c_o and L .

The initial and boundary conditions for Eq. (5) and (6) are

$$C_1(X, Y, Z, 0) = C_2(X, Y, Z, 0) = f(X, Y, Z) \quad (7)$$

$$(C_1 - \frac{1}{P_X} \frac{\partial C_1}{\partial X})|_{X=0^+} = g(Y, Z, T) \quad (8)$$

$$\frac{\partial C_1}{\partial X}(\infty, Y, Z, T) = 0 \quad (9)$$

$$C_1(X, \pm\infty, Z, T) = 0 \quad , \quad \frac{\partial C_1}{\partial Y}(X, \pm\infty, Z, T) = 0 \quad (10a,b)$$

$$C_1(X, Y, \pm\infty, T) = 0 \quad , \quad \frac{\partial C_1}{\partial Z}(X, Y, \pm\infty, T) = 0 \quad (11a,b)$$

where f and g are arbitrary functions which will be specified later, along with λ , to illustrate pertinent transport problems. Since advective-dispersive transport occurs exclusively in phase 1, the boundary conditions need to be cast in terms of C_1 .

Table 1. Dimensionless Parameters for the Two-Site and Two-Region Transport Models

Parameter	Two-site model	Two-region model
T	$\frac{vt}{L}$	$\frac{vt}{L}$
X, Y, Z	$\frac{x}{L}, \frac{y}{L}, \frac{z}{L}$	$\frac{x}{L}, \frac{y}{L}, \frac{z}{L}$
P_x, P_y, P_z	$\frac{vL}{D_x}, \frac{vL}{D_y}, \frac{vL}{D_z}$	$\frac{vL}{D_x}, \frac{vL}{D_y}, \frac{vL}{D_z}$
β	$\frac{\theta + f\rho k}{\theta + \rho k}$	$\frac{\theta_m + f\rho k}{\theta + \rho k}$
R	$1 + \frac{\rho k}{\theta}$	$1 + \frac{\rho k}{\theta}$
ω	$\frac{\alpha(1-\beta)RL}{v}$	$\frac{\alpha L}{\theta v}$
C_1	$\frac{c}{c_o}$	$\frac{c_m}{c_o}$
C_2	$\frac{s_k}{(1-f)kc_o}$	$\frac{c_{im}}{c_o}$
μ_1	$\frac{L}{\theta v} [\theta \mu_l + f \rho k \mu_{s,e}]$	$\frac{L}{\theta v} [\theta_m \mu_{l,m} + f \rho k \mu_{s,m}]$
μ_2	$\frac{L}{\theta v} [(1-f)\rho k \mu_{s,k}]$	$\frac{L}{\theta v} [\theta_{im} \mu_{l,im} + (1-f)\rho k \mu_{s,im}]$
λ_1	$\frac{L}{\theta v c_o} [\theta \lambda_l + f \rho \lambda_{s,e}]$	$\frac{L}{\theta v c_o} [\theta_m \lambda_{l,m} + f \rho \lambda_{s,m}]$
λ_2	$\frac{L}{\theta v c_o} [(1-f)\rho \lambda_{s,k}]$	$\frac{L}{\theta v c_o} [\theta_{im} \lambda_{l,im} + (1-f)\rho \lambda_{s,im}]$

The linearity of the problem makes it convenient to solve the boundary (BVP), initial (IVP), and production (PVP) value problems separately. According to the superposition principle, the solution to the overall transport problem is the sum of the individual solutions for the BVP, IVP, and PVP. In the BVP all conditions are homogeneous except for the input function, i.e., λ_1 and λ_2 in Eqs. (5) and (6), and $f(X, Y, Z)$ in Eq. (7) are equal to zero. The IVP is solved by having a zero input, $g(Y, Z, T)$, and no solute production. The PVP is based on a zero input and initial distribution. Similarly, subproblems can be solved independently within a BVP, IVP, or PVP. An example is a BVP involving the application of water of variable solute concentrations at different times.

Concentrations obtained from the effluent of finite soil columns, or from solution samplers, are usually viewed as representing the equilibrium concentration, C_1 . On the other hand, soil coring or nondestructive techniques such as TDR or electrical conductivity measurements will give total concentrations. The total resident concentration, C_T , is defined as the mass of solute per unit volume of soil, with weighted contributions from both the equilibrium (C_1) and nonequilibrium (C_2) phases according to:

$$C_T = \beta R C_1 + (1-\beta) R C_2 \quad (12)$$

The injection and detection modes employed in solute displacement experiments may require the use of flux-averaged or flowing concentrations [Kreft and Zuber, 1978; Parker and van Genuchten, 1984]. They can be obtained by substituting the analytical expression for the equilibrium or nonequilibrium resident concentration, C or C_R , obtained for a third-type inlet condition, into the well known transformation

$$C_F = C_R - \frac{1}{P_X} \frac{\partial C_R}{\partial X} \quad (13)$$

which is applicable because the simplicity of the flow and transport regime. The difference between C_F and C_R becomes quite small if P_X exceeds 5 [van Genuchten and Parker, 1984].

2.2. Derivation of Solutions

The solution of (5) and (6), subject to (7) through (11), was obtained using Laplace transforms with respect to X and T , and a double Fourier transform with respect to Y and Z [cf. Leij *et al.*, 1991; Toride *et al.*, 1993]. First, we apply the Laplace transform with respect to time:

$$\mathcal{L}_T[C(X, Y, Z, T)] = \bar{C}(X, Y, Z, s) = \int_0^\infty C(X, Y, Z, T) \exp(-sT) dT \quad (14)$$

with s as the transformation variable. Transformation of the problem yields [cf. *Spiegel*, 1965]:

$$\beta R(s\bar{C}_1 - f) = \frac{1}{P_X} \frac{\partial^2 \bar{C}_1}{\partial X^2} - \frac{\partial \bar{C}_1}{\partial X} + \frac{1}{P_Y} \frac{\partial^2 \bar{C}_1}{\partial Y^2} + \frac{1}{P_Z} \frac{\partial^2 \bar{C}_1}{\partial Z^2} + \omega(\bar{C}_2 - \bar{C}_1) - \mu_1 \bar{C}_1 + \frac{\lambda_1}{s} \quad (15)$$

$$(1 - \beta)R(s\bar{C}_2 - f) = \omega(\bar{C}_1 - \bar{C}_2) - \mu_2 \bar{C}_2 + \frac{\lambda_2}{s} \quad (16)$$

where we have used initial condition (7), while the remaining auxiliary conditions are

$$(\bar{C}_1 - \frac{1}{P_X} \frac{\partial \bar{C}_1}{\partial X})|_{X=0^+} = \bar{g}(Y, Z, s) \quad (17)$$

$$\frac{\partial \bar{C}_1}{\partial X} (\infty, Y, Z, s) = 0 \quad (18)$$

$$\bar{C}_1(X, \pm\infty, Z, s) = 0 \quad , \quad \frac{\partial \bar{C}_1}{\partial Y}(X, \pm\infty, Z, s) = 0 \quad (19a, b)$$

$$\bar{C}_1(X, Y, \pm\infty, s) = 0 \quad , \quad \frac{\partial \bar{C}_1}{\partial Z}(X, Y, \pm\infty, s) = 0 \quad (20a, b)$$

We can write the transport problem in terms of the equilibrium concentration by using the following relationship obtained by solving Eq. (16):

$$\bar{C}_2 = \frac{a_1 \bar{C}_1 + f + a_1 \lambda_2 / (\omega s)}{s + b} \quad (21)$$

where

$$a_1 = \frac{\omega}{(1 - \beta)R} \quad , \quad b = \frac{\omega + \mu_2}{(1 - \beta)R} \quad (22a, b)$$

It should be noted that for the regular time domain, the nonequilibrium concentration can be expressed in terms of the equilibrium concentration by inverting (21) using elementary properties of the Laplace transform:

$$C_2(X, Y, Z, T) = \frac{\omega}{(1-\beta)R} \int_0^T \exp[-b(T-\tau)] C_1(X, Y, Z, \tau) d\tau + f(X, Y, Z) \exp(-bT) + \frac{\lambda_2(X, Y, Z)}{\omega + \mu_2} [1 - \exp(-bT)] \quad (23)$$

where τ is a dummy integration variable — such dummy integration variables will be used frequently in this report. Substitution of (21) into (15) yields

$$\frac{1}{P_X} \frac{\partial^2 \bar{C}_1}{\partial X^2} - \frac{\partial \bar{C}_1}{\partial X} + \frac{1}{P_Y} \frac{\partial^2 \bar{C}_1}{\partial Y^2} + \frac{1}{P_Z} \frac{\partial^2 \bar{C}_1}{\partial Z^2} + \left(\frac{a_1 \omega}{s+b} - \omega - \mu_1 - \beta R s \right) \bar{C}_1 + \left(\frac{\omega}{s+b} + \beta R \right) f + \frac{\lambda_1}{s} + \frac{a_1 \lambda_2}{(s+b)s} = 0 \quad (24)$$

Since the problem is now expressed solely in terms of C_1 , we will drop the subscript as long as there is no need to distinguish between equilibrium and nonequilibrium concentrations.

Next, we use a Laplace transform with respect to X , i.e.:

$$\mathcal{L}_X [\bar{C}(X, Y, Z, s)] = \tilde{\bar{C}}(r, Y, Z, s) = \int_0^\infty \bar{C}(X, Y, Z, s) \exp(-rX) dX \quad (25)$$

where r denotes the Laplace variable for this particular transformation. Application of (25) to the above problem, and using inlet condition (17), leads to

$$\frac{1}{P_Y} \frac{\partial^2 \tilde{\bar{C}}}{\partial Y^2} + \frac{1}{P_Z} \frac{\partial^2 \tilde{\bar{C}}}{\partial Z^2} + \left(\frac{r^2}{P_X} - r + \frac{a_1 \omega}{s+b} - \omega - \mu_1 - \beta R s \right) \tilde{\bar{C}} + \bar{g} - \frac{r}{P_X} \bar{C}(0, Y, Z, s) + \left(\frac{\omega}{s+b} + \beta R \right) \tilde{f} + \frac{\tilde{\lambda}_1}{s} + \frac{a_1 \tilde{\lambda}_2}{(s+b)s} = 0 \quad (26)$$

subject to the conditions

$$\tilde{\bar{C}}(r, \pm\infty, Z, s) = 0 \quad , \quad \frac{\partial \tilde{\bar{C}}}{\partial Y}(r, \pm\infty, Z, s) = 0 \quad (27a,b)$$

$$\tilde{\bar{C}}(r, Y, \pm\infty, s) = 0 \quad , \quad \frac{\partial \tilde{\bar{C}}}{\partial Y}(r, Y, \pm\infty, s) = 0 \quad (28a,b)$$

Finally, we apply the double Fourier transform with respect to Y and Z , which is given by:

$$\mathcal{F}_{YZ} \left[\tilde{\tilde{C}}(r, Y, Z, s) \right] = \hat{\tilde{\tilde{C}}}(r, \gamma, \kappa, s) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp(i\gamma Y + i\kappa Z) \tilde{\tilde{C}}(r, Y, Z, s) dY dZ \quad (29)$$

where $i^2=-1$ and γ and κ are transformation variables pertaining to the Y and Z coordinates. If we transform (26) in this way, using (27) and (28), we can obtain the algebraic equation:

$$\hat{\tilde{\tilde{C}}}(r, \gamma, \kappa, s) = \frac{r \hat{\tilde{C}}(0, \gamma, \kappa, s) - P_X \left[\hat{g} + \left(\frac{\omega}{s+b} + \beta R \right) \hat{f} + \frac{\hat{\lambda}_1}{s} + \frac{a_1 \hat{\lambda}_2}{(s+b)s} \right]}{(r - r_+)(r - r_-)} \quad (30)$$

where

$$r_{\pm} = \frac{P_X}{2} \pm \sqrt{\frac{P_X^2}{4} - P_X \left(\frac{a_1 \omega}{s+b} - \omega - \mu_1 - \beta R s - \frac{\gamma^2}{P_Y} - \frac{\kappa^2}{P_Z} \right)} \quad (31)$$

This transformed solution in the Laplace and Fourier domains is not very useful; we need to apply inverse transformations to obtain results for the original time and space domains. We start with the inverse Laplace transform with respect to X . The right-hand side of Eq. (30) can be inverted term by term by using a table of Laplace transforms [cf. *Spiegel*, 1965] and, if needed, the convolution theorem. This process yields

$$\begin{aligned} \hat{\tilde{C}}(X, \gamma, \kappa, s) &= \frac{1}{r_- - r_+} \left\{ \left[r_- \exp(r_- X) - r_+ \exp(r_+ X) \right] \hat{\tilde{C}}(0, \gamma, \kappa, s) - \left[\exp(r_- X) - \exp(r_+ X) \right] P_X \hat{g} \right. \\ &\quad \left. - P_X \int_0^X \left[\exp[r_-(X-\xi)] - \exp[r_+(X-\xi)] \right] \left[\left(\frac{\omega}{s+b} + \beta R \right) \hat{f}(\xi) + \frac{\hat{\lambda}_1(\xi)}{s} + \frac{a_1 \hat{\lambda}_2(\xi)}{(s+b)s} \right] d\xi \right\} \end{aligned} \quad (32)$$

We have used all conditions except the outlet condition, i.e., Eq. (9) in the regular space-time domain. If we differentiate (32) and use Leibniz' rule for the differentiation of an integral, we can determine the following equality:

$$\begin{aligned} \frac{d\hat{\bar{C}}}{dX}(\infty, \gamma, \kappa, s) &= -\hat{\bar{C}}(0, \gamma, \kappa, s) + \frac{P_X \hat{g}}{r_+} \\ &\quad + \frac{P_X}{r_+} \int_0^\infty \exp(-r_+ \xi) \left[\left(\frac{\omega}{s+b} + \beta R \right) \hat{f}(\xi) + \frac{\hat{\lambda}_1(\xi)}{s} + \frac{a_1 \hat{\lambda}_2(\xi)}{(s+b)s} \right] d\xi = 0 \end{aligned} \quad (33)$$

After substituting the resulting expression for $\hat{\bar{C}}(0, \gamma, \kappa, s)$ in (32), we can write the solution as the sum of solutions to the BVP, IVP and PVP:

$$\begin{aligned} \hat{\bar{C}}(X, \gamma, \kappa, s) &= \frac{P_X \hat{g}}{r_+} \exp(r_- X) \\ &\quad + \frac{P_X}{r_- - r_+} \left(\frac{\omega}{s+b} + \beta R \right) \left\{ \frac{r_-}{r_+} \exp(P_X X) \int_0^\infty \exp[-r_+(X+\xi)] \hat{f}(\xi) d\xi \right. \\ &\quad \left. - \int_X^\infty \exp[r_+(X-\xi)] \hat{f}(\xi) d\xi - \int_0^X \exp[r_-(X-\xi)] \hat{f}(\xi) d\xi \right\} \\ &\quad + \frac{P_X}{r_- - r_+} \left\{ \frac{r_+}{r_-} \exp(P_X X) \int_0^\infty \exp[-r_+(X+\xi)] \left[\frac{\hat{\lambda}_1(\xi)}{s} + \frac{a_1 \hat{\lambda}_2(\xi)}{(s+b)s} \right] d\xi \right. \\ &\quad \left. - \int_X^\infty \exp[r_+(X-\xi)] \left[\frac{\hat{\lambda}_1(\xi)}{s} + \frac{a_1 \hat{\lambda}_2(\xi)}{(s+b)s} \right] d\xi - \int_0^X \exp[r_-(X-\xi)] \left[\frac{\hat{\lambda}_1(\xi)}{s} + \frac{a_1 \hat{\lambda}_2(\xi)}{(s+b)s} \right] d\xi \right\} \end{aligned} \quad (34)$$

The next step is the inversion with respect to time. We rewrite (31) as [cf. *Villermaux and van Swaaij, 1969; Toride et al., 1993*]

$$r_\pm = \frac{P_X}{2} \pm a_0 \sqrt{s+b - \frac{a_2}{s+b} + d} \quad (35)$$

with

$$a_0 = \sqrt{\beta R P_X}, \quad a_2 = \frac{\omega}{\beta R} a_1 = \frac{\omega^2}{(1-\beta)\beta R^2}, \quad d = \frac{1}{\beta R} \left(\frac{P_X}{4} + \frac{\gamma^2}{P_Y} + \frac{\kappa^2}{P_Z} + \omega + \mu_1 \right) - b \quad (36a,b,c)$$

The inversion is based on the property that the iterated Laplace transform of a function is equal to the generalized convolution integral of the function. The following identities will be used [cf. *De*

Smedt and Wierenga, 1979a; Lindstrom and Stone, 1974:

$$\mathcal{L}_T \left\{ \exp(-bT) \int_0^T I_0 [2\sqrt{a_2(T-\tau)} \tau] h(\tau) d\tau \right\} = \frac{1}{s+b} \bar{h}\left(s+b - \frac{a_2}{s+b}\right) = \frac{\bar{h}(s^*)}{s+b} \quad (37)$$

$$\mathcal{L}_T \left\{ \exp(-bT) \frac{\partial}{\partial T} \int_0^T I_0 [2\sqrt{a_2(T-\tau)} \tau] h(\tau) d\tau \right\} = \bar{h}\left(s+b - \frac{a_2}{s+b}\right) = \bar{h}(s^*) \quad (38)$$

where I_0 is the modified Bessel function of order zero while $h(\tau)$ and $\bar{h}(s^*)$ denote an arbitrary function in the regular time and Laplace domains, respectively, with $s^* = s+b-a_2/(s+b)$. We will continue by deriving general solutions for the BVP, IVP, and PVP.

2.2.1. Boundary Value Problem

The solution of the BVP, the first term on the right-hand side of (34), may be expressed as

$$\hat{C}(X, \gamma, \kappa, s) = \frac{P_X g(s)}{a_0} \exp\left(\frac{P_X X}{2}\right) \bar{h}_1(X, s^* + d) \quad (39)$$

The inversion with respect to time is carried out using (38); subsequent integration yields

$$\begin{aligned} \hat{C}(X, \gamma, \kappa, T) &= \frac{P_X}{a_0} \exp\left(\frac{P_X X}{2}\right) \int_0^T \hat{g}(T-\tau) \exp(-b\tau) \\ &\times \left(h_1(X, \tau) + \int_0^\tau \sqrt{\frac{a_2 \eta}{\tau-\eta}} I_1[2\sqrt{a_2(\tau-\eta)}\eta] h_1(X, \eta) d\eta \right) d\tau \end{aligned} \quad (40)$$

where I_1 denotes the modified first-order Bessel functions, while η and τ represent dummy variables. The expressions for the transformed and inverse function h are

$$\bar{h}_1(X, s^* + d) = \exp\left(-a_0 X \sqrt{s^* + d}\right) / \left(\frac{P_X}{2a_0} + \sqrt{s^* + d}\right) \quad (41)$$

$$h_1(X, \tau) = \exp(-dt) \left[\frac{1}{\sqrt{\pi\tau}} \exp\left(-\frac{a_0^2 X^2}{4\tau}\right) - \frac{P_X}{2a_0} \exp\left(\frac{P_X^2 \tau}{4a_0^2} + \frac{P_X X}{2}\right) \operatorname{erfc}\left(\frac{a_0^2 X + P_X \tau}{2a_0 \sqrt{\tau}}\right) \right] \quad (42)$$

We also need to apply the inverse Fourier transform. Inversion of the part of (40) that depends on γ and κ is accomplished with the convolution theorem according to

$$\begin{aligned} \mathcal{F}_{YZ}^{-1} \left\{ \hat{g}(T-\tau) \exp \left[-\frac{\tau}{\beta R} \left(\frac{\gamma^2}{P_Y} + \frac{\kappa^2}{P_Z} \right) \right] \right\} &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(T-\tau, Y-\varphi, Z-\Omega) \Gamma(\varphi, \Omega, \tau) d\varphi d\Omega \\ &= \frac{\beta R \sqrt{P_Y P_Z}}{4\pi\tau} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(T-\tau, Y-\varphi, Z-\Omega) \exp \left[-\frac{\beta R (P_Y \varphi^2 + P_Z \Omega^2)}{4\tau} \right] d\varphi d\Omega \end{aligned} \quad (43)$$

where φ and Ω are dummy variables and $\Gamma(\varphi, \Omega, \tau)$ is an auxiliary transverse function. The latter function can be evaluated further depending on the transverse distribution of the input function, as will be discussed in section 3.3.

We can now obtain the equilibrium concentration in the regular space-time domain. The nonequilibrium concentration follows from (23). For an arbitrary input function, $g(Y, Z, T)$, the general solution to the BVP is

$$\begin{aligned} C_1(X, Y, Z, T) &= \int_0^T \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(Y-\varphi, Z-\Omega, T-\tau) \left[\exp \left(-\frac{\omega\tau}{\beta R} \right) \Gamma(\varphi, \Omega, \tau) G(X, \tau) \right. \\ &\quad \left. + \int_0^{\tau} \sqrt{\frac{a_2 \eta}{\tau-\eta}} H_1(\eta, \tau) \Gamma(\varphi, \Omega, \eta) G(X, \eta) d\eta \right] d\Omega d\varphi d\tau \end{aligned} \quad (44)$$

$$C_2(X, Y, Z, T) = \frac{\omega}{(1-\beta)R} \int_0^T \exp \left(-\frac{\omega+\mu_2}{(1-\beta)R} (T-\tau) \right) C_1(X, Y, Z, \tau) d\tau \quad (45)$$

The auxiliary longitudinal function for the BVP, $G(X, \tau)$, is defined in Table 2. The auxiliary nonequilibrium function is

$$H_n(\tau, T) = \exp \left(-\frac{\omega\tau}{\beta R} - \frac{\omega+\mu_2}{(1-\beta)R} (T-\tau) \right) I_n[2\sqrt{a_2(T-\tau)\tau}] \quad (n = 0, 1) \quad (46)$$

The longitudinal dependency of the solution is completely contained in the term G . This feature allows for a convenient transformation from resident to flux-averaged concentrations according to Eq. (13). Expressions for $G(X, \tau)$ to be used in conjunction with resident and flux-averaged concentrations are given in Tables 2a and 2b, respectively, at the end of this chapter.

2.2.2. Initial Value Problem

The solution for the IVP is a bit longer than for the BVP, but the inversion to the regular time domain follows the same pattern. The second part of the right-hand side of Eq. (34) can be rewritten as

$$\begin{aligned} \hat{\bar{C}}_1(X, \gamma, \kappa, s) &= \frac{P_X}{2a_0} \left(\frac{\omega}{s+b} + \beta R \right) \\ &\times \left\{ \int_0^\infty \left[\bar{h}_1(X+\xi, s^*+d) - \frac{P_X}{2a_0} \bar{h}_2(X+\xi, s^*+d) \right] \exp \left[\frac{P_X}{2}(X-\xi) \right] \hat{f}(\xi) d\xi \right. \\ &+ \int_X^\infty \bar{h}_3(\xi-X, s^*+d) \exp \left[\frac{P_X}{2}(X-\xi) \right] \hat{f}(\xi) d\xi \\ &\left. + \int_0^X \bar{h}_3(X-\xi, s^*+d) \exp \left[\frac{P_X}{2}(X-\xi) \right] \hat{f}(\xi) d\xi \right\} \end{aligned} \quad (47)$$

The inversion is conducted with the aid of (37) and (38) to obtain

$$\begin{aligned} \hat{\bar{C}}(X, \gamma, \kappa, T) &= \frac{P_X}{2a_0} \int_0^\infty \left\{ \omega \int_0^T I_0 \left[2\sqrt{a_2(T-\tau)} \right] \left[h_1(X+\xi, \tau) - \frac{P_X}{2a_0} h_2(X+\xi, \tau) + h_3(\xi-X, \tau) \right] d\tau \right. \\ &+ \beta R \frac{\partial}{\partial \tau} \int_0^T \left(I_0 \left[2\sqrt{a_2(T-\tau)} \right] \left[h_1(X+\xi, \tau) - \frac{P_X}{2a_0} h_2(X+\xi, \tau) + h_3(\xi-X, \tau) \right] d\tau \right) \left. \right\} \\ &\times \exp \left[-bT - \frac{P_X}{2}(X-\xi) \right] \hat{f}(\xi) d\xi \end{aligned} \quad (48)$$

where $\bar{h}_1(X, s^*+d)$ and $h_1(X, \tau)$ are the same as defined earlier by (41) and (42), and where

$$\bar{h}_2(X, s^*+d) = \frac{\exp(-a_0 X \sqrt{s^*+d})}{\left(\frac{P_X}{2a_0} + \sqrt{s^*+d} \right) \sqrt{s^*+d}} \quad (49)$$

$$h_2(X, T) = \exp \left(-dT + \frac{P_X^2 T}{4a_0^2} + \frac{P_X X}{2} \right) \operatorname{erfc} \left(\frac{a_0^2 X + P_X T}{2a_0 \sqrt{T}} \right) \quad (50)$$

$$\bar{h}_3(X, s^* + d) = \frac{\exp(-a_0 X \sqrt{s^* + d})}{\sqrt{s^* + d}} \quad (51)$$

$$h_3(X, T) = \frac{1}{\sqrt{\pi T}} \exp\left(-dT - \frac{a_0^2 X^2}{4T}\right) \quad (52)$$

If we carry out the differentiation in (48) and apply the Fourier inversion according to (43), we may obtain the following equilibrium and nonequilibrium solutions:

$$C_1(X, Y, Z, T) = \int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty f(\xi, Y - \varphi, Z - \Omega) \left[\exp\left(-\frac{\omega T}{\beta R}\right) \Gamma(\varphi, \Omega, T) G(\xi, T; X) \right. \\ \left. + \int_0^T \left(\frac{\omega}{\beta R} H_0(\tau, T) + \sqrt{\frac{a_2 \tau}{T - \tau}} H_1(\tau, T) \right) \Gamma(\varphi, \Omega, \tau) G(\xi, \tau; X) d\tau \right] d\omega d\varphi d\xi \quad (53)$$

$$C_2(X, Y, Z, T) = f(X, Y, Z) \exp\left(-\frac{\omega + \mu_2}{(1-\beta)R} T\right) + \frac{\omega}{(1-\beta)R} \int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty \int_0^T f(\xi, Y - \varphi, Z - \Omega) \\ \times \left(H_0(\tau, T) + \sqrt{\frac{(1-\beta)(T-\tau)}{\beta\tau}} H_1(\tau, T) \right) \Gamma(\varphi, \Omega, \tau) G(\xi, \tau; X) d\tau d\Omega d\varphi d\xi \quad (54)$$

where $G(\xi, \tau; X)$ and $\Gamma(\varphi, \Omega, \tau)$ are as defined in Table 2 and 3, while $H_0(\tau; T)$ is given by Eq. (46).

2.2.3 Production Value Problem

The Laplace transform of the solution for the PVP can be written as (cf. Eq. (34)):

$$\begin{aligned}\hat{A}(X, \gamma, \kappa, s) = & \frac{P_X}{2a_0} \int_0^\infty \left[\bar{h}_1(X + \xi, s^* + d) - \frac{P_X}{2a_0} \bar{h}_2(X + \xi, s^* + d) \right] \exp\left[\frac{P_X}{2}(X - \xi)\right] \left[\frac{\hat{\lambda}_1(\xi)}{s} + \frac{a_1 \hat{\lambda}_2(\xi)}{s(s+b)} \right] d\xi \\ & + \frac{P_X}{2a_0} \int_X^\infty \bar{h}_3(\xi - X, s^* + d) \exp\left[\frac{P_X}{2}(X - \xi)\right] \left[\frac{\hat{\lambda}_1(\xi)}{s} + \frac{a_1 \hat{\lambda}_2(\xi)}{s(s+b)} \right] d\xi \\ & + \frac{P_X}{2a_0} \int_0^X \bar{h}_3(X - \xi, s^* + d) \exp\left[\frac{P_X}{2}(X - \xi)\right] \left[\frac{\hat{\lambda}_1(\xi)}{s} + \frac{a_1 \hat{\lambda}_2(\xi)}{s(s+b)} \right] d\xi\end{aligned}\quad (55)$$

The solution procedure is very similar as for the IVP. Hence we proceed by stating the solution for the equilibrium and nonequilibrium concentration in case of unspecified zero-order production terms:

$$\begin{aligned}C_1(X, Y, Z, T) = & \frac{1}{\beta R} \int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty \int_0^T \left[\lambda_1(\xi, Y - \varphi, Z - \Omega) \exp\left(-\frac{\omega\tau}{\beta R}\right) \Pi(\varphi, \Omega, \tau) G(\xi, \tau, X) \right. \\ & + \int_0^\tau \left(a_1 H_0(\eta, \tau) \lambda_2(\xi, Y - \varphi, Z - \Omega) + \sqrt{\frac{a_2 \eta}{\tau - \eta}} H_1(\eta, \tau) \lambda_1(\xi, Y - \varphi, Z - \Omega) \right) \\ & \times \left. \Pi(\varphi, \Omega, \eta) G(\xi, \eta, X) d\eta \right] d\tau d\Omega d\varphi d\xi\end{aligned}\quad (56)$$

$$C_2(X, Y, Z, T) = \frac{\lambda_2(X, Y, Z)}{\omega + \mu_2} [1 - \exp(-bT)] + \frac{\omega}{(1 - \beta)R} \int_0^T \exp[-b(T - \tau)] C_1(X, Y, Z, \tau) d\tau \quad (57)$$

where the same auxiliary functions have been used as for the IVP. The solution of the PVP may alternatively be expressed in terms of Goldstein's J -function. This function will also appear in the specific solutions given in Chapter 3. Hence, we will discuss Goldstein's J -function in somewhat more detail.

The above expressions may be simplified by evaluating the integral with respect to τ in (56). We change the order of integration according to Fubini's theorem [cf. *Lindstrom and Stone, 1974*]

$$\int_0^T \int_0^\tau f(\eta, \tau) d\eta d\tau = \int_0^T \int_\eta^T f(\eta, \tau) d\tau d\eta \quad (58)$$

to rewrite (56) as

$$\begin{aligned}
 C_1(X, Y, Z, T) = & \frac{1}{\beta R} \int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty \left[\int_0^T \exp\left(-\frac{\omega\tau}{\beta R}\right) \lambda_1(\xi, Y-\varphi, Z-Q) I(\varphi, Q, \tau) G(\xi, \tau, X) d\tau \right. \\
 & + \int_0^T \int_\eta^T \exp\left(-p' - \frac{\omega\mu_2\eta}{(\omega+\mu_2)\beta R} - q'\right) \left(\lambda_1(\xi, Y-\varphi, Z-Q) \frac{\omega+\mu_2}{(1-\beta)R} \sqrt{\frac{p'}{q'}} I_1[2\sqrt{p'q'}] \right. \\
 & \left. \left. + a_2 \lambda_2(\xi, Y-\varphi, Z-Q) I_0[2\sqrt{p'q'}] \right) \Gamma(\varphi, Q, \eta) G(\xi, \eta, X) d\tau d\eta \right] dQ d\varphi d\xi
 \end{aligned} \quad (59)$$

where

$$p' = \frac{\omega^2}{(\omega+\mu_2)\beta R} \eta \quad , \quad q' = \frac{\omega+\mu_2}{(1-\beta)R} (\tau - \eta) \quad (60a,b)$$

The second integral with respect to τ in (59), is rewritten with the J -function [Goldstein, 1953]:

$$J(p, q) = 1 - \exp(-q) \int_0^p \exp(-w) I_0[2\sqrt{qw}] dw \quad (61)$$

with w as dummy variable and

$$p = \frac{\omega^2}{(\omega+\mu_2)\beta R} \tau \quad , \quad q = \frac{\omega+\mu_2}{(1-\beta)R} (T - \tau) \quad (62a,b)$$

With the help of (60b) and the properties

$$\frac{\partial J(p, q)}{\partial q} = \exp(-p - q) \sqrt{\frac{p}{q}} I_1[2\sqrt{pq}] \quad , \quad J(p, 0) = \exp(-p) \quad (63a,b)$$

we can establish that

$$\int_\eta^T \frac{\omega+\mu_2}{(1-\beta)R} \exp(-p' - q') \sqrt{\frac{p'}{q'}} I_1(2\sqrt{p'q'}) d\tau = J(p', q'') - \exp(-p') \quad (64)$$

$$\int_\eta^T \exp(-p' - q') I_0(2\sqrt{p'q'}) d\tau = \frac{\omega+\mu_2}{(1-\beta)R} [1 - J(q'', p')] \quad (65)$$

where

$$q'' = \frac{\omega+\mu_2}{(1-\beta)R} (T - \eta) \quad (66)$$

The equilibrium concentration can now be simplified to

$$C_1(X, Y, Z, T) = \frac{1}{\beta R} \int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty \int_0^T \exp\left(-\frac{\omega\mu_2\tau}{(\omega+\mu_2)\beta R}\right) \\ \times \left(\lambda_1(\xi, Y-\varphi, Z-\Omega) J(p, q) + \frac{\omega\lambda_2(\xi, Y-\varphi, Z-\Omega)}{\omega+\mu_2} [1-J(p, q)] \right) G(\xi, \tau, X) d\tau d\varphi d\Omega d\xi \quad (67)$$

The nonequilibrium concentration is derived by substituting (67) into (57). The resulting double integration with respect to τ and η is simplified with Fubini's theorem and integration by parts. With help of the chain rule we can establish that:

$$\frac{\partial J(p', q')}{\partial \tau} = \frac{\omega+\mu_2}{(1-\beta)R} \exp(-p' - q') \sqrt{\frac{p'}{q'}} I_1[2\sqrt{p'q'}] \quad (68)$$

$$\frac{\partial J(q', p')}{\partial \tau} = -\frac{\omega+\mu_2}{(1-\beta)R} \exp(-p' - q') I_0[2\sqrt{p'q'}] \quad (69)$$

while integration by parts gives

$$\int_\eta^T \sqrt{\frac{p'}{q'}} I_1(2\sqrt{p'q'}) d\tau = \frac{(1-\beta)R}{\omega+\mu_2} [I_0(2\sqrt{p'q''}) - 1] \quad (70)$$

$$\int_\eta^T I_0(2\sqrt{p'q'}) d\tau = \sqrt{\frac{q''}{p'}} I_1(2\sqrt{p'q''}) \quad (71)$$

The following expression may now be established for the nonequilibrium concentration:

$$C_2(X, Y, Z, T) = \frac{\lambda_2(X, Y, Z)}{\omega+\mu_2} \left[1 - \exp\left(-\frac{\omega+\mu_2}{(1-\beta)R} T\right) \right] \\ + \frac{\omega}{\beta R (\omega+\mu_2)} \int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty \int_0^T \exp\left(-\frac{\omega\mu_2\tau}{(\omega+\mu_2)\beta R}\right) \\ \times \left\{ \lambda_1(\xi, Y-\varphi, Z-\Omega) [J(p, q) - \exp(-p-q) I_0(2\sqrt{pq})] \right. \\ \left. + \frac{\omega\lambda_2(\xi, Y-\varphi, Z-\Omega)}{\omega+\mu_2} [1-J(q, p) + \sqrt{\frac{q}{p}} \exp(-p-q) I_1(2\sqrt{pq})] \right\} \\ I(Y-\varphi, Z-\Omega) G(\xi, \tau, X) d\tau d\varphi d\Omega d\xi \quad (72)$$

Table 2a. Expressions for the Auxiliary Longitudinal Term, G , in General and Specific Solutions to the BVP, IVP, and PVP for Resident Concentrations

G	Expression
$G(X, \tau)$	$\exp\left(-\frac{\mu_1 \tau}{\beta R}\right) \left[\sqrt{\frac{P_X}{\pi \beta R \tau}} \exp\left(-\frac{(\beta R X - \tau)^2}{4 \beta R \tau / P_X}\right) \right.$ $\left. - \frac{P_X}{2 \beta R} \exp(P_X X) \operatorname{erfc}\left(\frac{\beta R X + \tau}{\sqrt{4 \beta R \tau / P_X}}\right) \right]$
$G(\xi, \tau; X)$	$\exp\left(-\frac{\mu_1 \tau}{\beta R}\right) \left[\sqrt{\frac{\beta R P_X}{4 \pi \tau}} \exp\left(P_X X - \frac{[\beta R(\xi + X) + \tau]^2}{4 \beta R \tau / P_X}\right) \right.$ $- \frac{P_X}{2} \exp(P_X X) \operatorname{erfc}\left(\frac{\beta R(\xi + X) + \tau}{\sqrt{4 \beta R \tau / P_X}}\right)$ $\left. + \sqrt{\frac{\beta R P_X}{4 \pi \tau}} \exp\left(-\frac{[\beta R(\xi - X) + \tau]^2}{4 \beta R \tau / P_X}\right) \right]$
$G_1(X, \tau; X_i)$	$\exp\left(-\frac{\mu_1 \tau}{\beta R}\right) \left[1 - \frac{1}{2} \operatorname{erfc}\left(\frac{\beta R(X - X_i) - \tau}{\sqrt{4 \beta R \tau / P_X}}\right) \right.$ $+ \frac{1}{2} \left(1 + P_X(X + X_i) + \frac{P_X \tau}{\beta R} \right) \exp(P_X X) \operatorname{erfc}\left(\frac{\beta R(X + X_i) + \tau}{\sqrt{4 \beta R \tau / P_X}}\right)$ $\left. - \sqrt{\frac{P_X \tau}{\pi \beta R}} \exp\left(P_X X - \frac{[\beta R(X + X_i) + \tau]^2}{4 \beta R \tau / P_X}\right) \right]$
$G_2(X, \tau; \alpha)$	$\exp\left((\alpha + \alpha^2 / P_X - \mu_1) \frac{\tau}{\beta R}\right)$ $\times \left\{ \exp(-\alpha X) \left[1 - \frac{1}{2} \operatorname{erfc}\left(\frac{\beta R X - \tau(1 + 2 \alpha / P_X)}{\sqrt{4 \beta R \tau / P_X}}\right) \right] \right.$ $+ \frac{1}{2} (1 + P_X / \alpha) \exp[(\alpha + P_X) X] \operatorname{erfc}\left[\frac{\beta R X + \tau(1 + 2 \alpha / P_X)}{\sqrt{4 \beta R \tau / P_X}}\right] \left. \right\}$ $- \frac{P_X}{2 \alpha} \exp(P_X X - \frac{\mu_1 \tau}{\beta R}) \operatorname{erfc}\left[\frac{\beta R X + \tau}{\sqrt{4 \beta R \tau / P_X}}\right]$

Table 2b. Expressions for the Auxiliary Longitudinal Term, G , in General and Specific Solutions to the BVP, IVP, and PVP for Flux-Averaged Concentrations

G	Expression
$G(X, \tau)$	$\sqrt{\frac{\beta R P_X X^2}{4\pi \tau^3}} \exp\left(-\frac{\mu_1 \tau}{\beta R} - \frac{(\beta R X - \tau)^2}{4\beta R \tau / P_X}\right)$
$G(\xi, \tau; X)$	$\sqrt{\frac{\beta R P_X}{4\pi \tau}} \exp\left(-\frac{\mu_1 \tau}{\beta R}\right) \left[[1 - \frac{\beta R(\xi - X) + \tau}{2\tau}] \exp\left(-\frac{[\beta R(\xi - X) + \tau]^2}{4\beta R \tau / P_X}\right) \right. \\ \left. - [1 - \frac{\beta R(\xi + X) + \tau}{2\tau}] \exp\left(P_X X - \frac{[\beta R(\xi + X) + \tau]^2}{4\beta R \tau / P_X}\right) \right]$
$G_1(X, \tau; X_i)$	$\exp\left(-\frac{\mu_1 \tau}{\beta R}\right) \left\{ 1 - \frac{1}{2} \operatorname{erfc}\left[\frac{\beta R(X - X_i) - \tau}{\sqrt{4\beta R \tau / P_X}}\right] \right. \\ \left. - \frac{1}{2} \exp(P_X X) \operatorname{erfc}\left[\frac{\beta R(X + X_i) + \tau}{\sqrt{4\beta R \tau / P_X}}\right] \right. \\ \left. - \sqrt{\frac{\beta R}{4\pi \tau P_X}} \exp\left(-\frac{[\beta R(X - X_i) - \tau]^2}{4\beta R \tau / P_X}\right) \right. \\ \left. + \sqrt{\frac{\beta R}{4\pi \tau P_X}} \exp\left(P_X X - \frac{[\beta R(X + X_i) + \tau]^2}{4\beta R \tau / P_X}\right) \right\}$
$G_2(X, \tau; \alpha)$	$(1 + \frac{\alpha}{P_X}) \exp\left((\alpha + \alpha^2 / P_X - \mu_1) \frac{\tau}{\beta R}\right) \\ \left\{ \exp(-\alpha X) \left[1 - \frac{1}{2} \operatorname{erfc}\left(\frac{\beta R X - \tau(1 + 2\alpha/P_X)}{\sqrt{4\beta R \tau / P_X}}\right) \right] \right. \\ \left. + \frac{1}{2} \exp[(\alpha + P_X)X] \operatorname{erfc}\left[\frac{\beta R X + \tau(1 + 2\alpha/P_X)}{\sqrt{4\beta R \tau / P_X}}\right] \right\}$

Table 3. Expressions for the Transverse Term, Γ , in General and Specific Solutions to the BVP, IVP, and PVP

Γ	Expression
$\Gamma(\varphi, \Omega, T) = \Gamma_Y(\varphi, T)\Gamma_Z(\Omega, T)$	$\frac{\beta R \sqrt{P_Y P_Z}}{4\pi T} \exp\left(-\frac{\beta R(P_Y \varphi^2 + P_Z \Omega^2)}{4T}\right)$
$\Gamma_1(Y, T), \Gamma_1(Z, T)$	$\sqrt{\frac{\beta R P_Y}{4\pi T}} \exp\left(-\frac{\beta R P_Y Y^2}{4T}\right), \quad \sqrt{\frac{\beta R P_Z}{4\pi T}} \exp\left(-\frac{\beta R P_Z Z^2}{4T}\right)$
$\Gamma_2(Y, T; Y_i)$	$\frac{1}{2} \operatorname{erfc}\left(\sqrt{\frac{\beta R P_Y}{4T}}(Y - Y_i)\right)$
$\Gamma_3(Y, T; Y_0)$	$\begin{aligned} &\frac{1}{2} \exp\left(\alpha(Y_0 - Y) + \frac{\alpha^2 T}{\beta R P_Y}\right) \operatorname{erfc}\left(\frac{\beta R P_Y(Y_0 - Y) + 2\alpha T}{4\beta R P_Y T}\right) \\ &+ \frac{1}{2} \exp\left(\alpha(Y - Y_0) + \frac{\alpha^2 T}{\beta R P_Y T}\right) \operatorname{erfc}\left(\frac{\beta R P_Y(Y - Y_0) + 2\alpha T}{4\beta R P_Y T}\right) \end{aligned}$
$\Gamma_4(Y, Z, T; r_i)$	$\begin{aligned} &\frac{1}{2} \int_{Y-r_i}^{Y+r_i} \sqrt{\frac{\beta R P_Y}{4\pi T}} \exp\left(-\frac{\beta R P_Y \varphi^2}{4T}\right) \left\{ \operatorname{erfc}\left[\sqrt{\frac{\beta R P_Z}{4T}}\left(Z - \sqrt{r_i^2 - (Y - \varphi)^2}\right)\right] \right. \\ &\quad \left. - \operatorname{erfc}\left[\sqrt{\frac{\beta R P_Z}{4T}}\left(Z + \sqrt{r_i^2 - (Y - \varphi)^2}\right)\right] \right\} d\varphi \end{aligned}$
$\Gamma_5(Y, Z, T)$	$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\beta R \sqrt{P_Y P_Z}}{4\pi T} \exp\left(-\alpha\sqrt{(Y - \varphi)^2 + (Z - \Omega)^2} - \frac{\beta R}{4T}(P_Y \varphi^2 + P_Z \Omega^2)\right) d\Omega d\varphi$
$\Gamma_6(\xi, Y, Z, T; r_i, X_0)$	$\begin{aligned} &\frac{1}{2} \int_{Y - \sqrt{r_i^2 - (\xi - X_0)^2}}^{Y + \sqrt{r_i^2 - (\xi - X_0)^2}} \sqrt{\frac{\beta R P_Y}{4\pi T}} \exp\left(-\frac{\beta R P_Y \varphi^2}{4T}\right) \\ &\times \left[\operatorname{erfc}\left(\sqrt{\frac{\beta R P_Z}{4T}}[Z - \sqrt{r_i^2 - (\xi - X_0)^2} - (Y - \varphi)^2]\right) \right. \\ &\quad \left. - \operatorname{erfc}\left(\sqrt{\frac{\beta R P_Z}{4T}}[Z + \sqrt{r_i^2 - (\xi - X_0)^2} - (Y - \varphi)^2]\right) \right] d\varphi \end{aligned}$
$\Gamma_7(Y, Z, T)$	$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\beta R \sqrt{P_Y P_Z}}{4\pi T} \exp\left(-\alpha\sqrt{(\xi - X_0)^2 + (Y - \varphi)^2 + (Z - \Omega)^2} - \frac{\beta R}{4T}(P_Y \varphi^2 + P_Z \Omega^2)\right) d\Omega d\varphi$

3. SPECIFIC SOLUTIONS

In this chapter we will use the general solutions of Chapter 2 to derive specific analytical solutions. For the input function, g , the initial profile, f , and the production curve, λ , we will assume relatively simple Dirac, Heaviside, and exponential functions. The auxiliary mathematical conditions are given as the product of terms that each depend on a different independent variable (i.e., X or T , Y , and Z). This approach will be illustrated briefly in section 3.1. The specific solutions may be written as a combination of longitudinal and transversal subsolutions. Longitudinal subsolutions will be presented in sections 3.2.1 through 3.2.3, whereas the transverse subsolution is discussed in section 3.2.4. We note that the input function can be specified over rectangular and circular areas of the YZ -plane, whereas the initial and production profiles may also be specified for rectangular or circular regions of the XYZ -space. The part of the solution that depends on X will be specified in section 3.2.1 for the BVP, in section 3.2.2 for the IVP, and in section 3.2.3. for the IVP; the part of the solution that depends on the transversal (radial) distance is defined in section 3.2.4. Conditions for the IVP and PVP may also be specified over spherical regions. The complete problem and the solution for this case are presented in sections 3.2.2 and 3.2.3, respectively. All conditions for which N3DADE evaluates the solution are listed in section 3.3.

3.1. Input, Initial, and Production Profiles

The input, initial and production profiles are written as the product of terms that depend on a single variable:

$$g(Y, Z, T) = g_T(T) g_Y(Y) g_Z(Z) \quad (73)$$

$$f(X, Y, Z) = f_X(X) f_Y(Y) f_Z(Z) \quad (74)$$

$$\lambda_k(X, Y, Z) = \lambda_{kX}(X) \lambda_{kY}(Y) \lambda_{kZ}(Z) \quad (k = 1, 2) \quad (75)$$

The right-hand side of the above expressions consists of one longitudinal and two transversal terms, respectively. The longitudinal term would also be encountered for one-dimensional problems, i.e., the input concentration, g_T , as a function of time, T , for the BVP; the initial distribution, f_X , as a

function of longitudinal distance, X , for the IVP; and solute production in regions 1 and 2, λ_{1X} and λ_{2X} , as a function of X for the PVP. Each longitudinal and transversal term is specified independently as a Dirac, Heaviside, or an exponential function. All problems are solved for a Cartesian coordinate system. However, only one function can be chosen to specify the problem in the transverse direction for a circular region, whereas for spherical regions only one function can be selected for the problem.

The use of the Dirac, Heaviside, and exponential functions for the longitudinal term is illustrated schematically in Figure 1. The Dirac function is used to describe the application of a finite amount of solute over an infinitely small temporal or spatial interval. No Dirac function is used to model solute production. The Heaviside function is used for the BVP, IVP, and PVP to describe profiles where a step change in value occurs at a finite number of times or positions. The illustration for the PVP pertains to a production rate λ_{11} in the equilibrium phase and λ_{21} in the nonequilibrium phase for $X < X_2$; for $X > X_2$ these rates are given by the respective constants λ_{12} and λ_{22} . Finally, the exponential function quantifies an exponential decrease in concentration or solute production as a function of time or position.

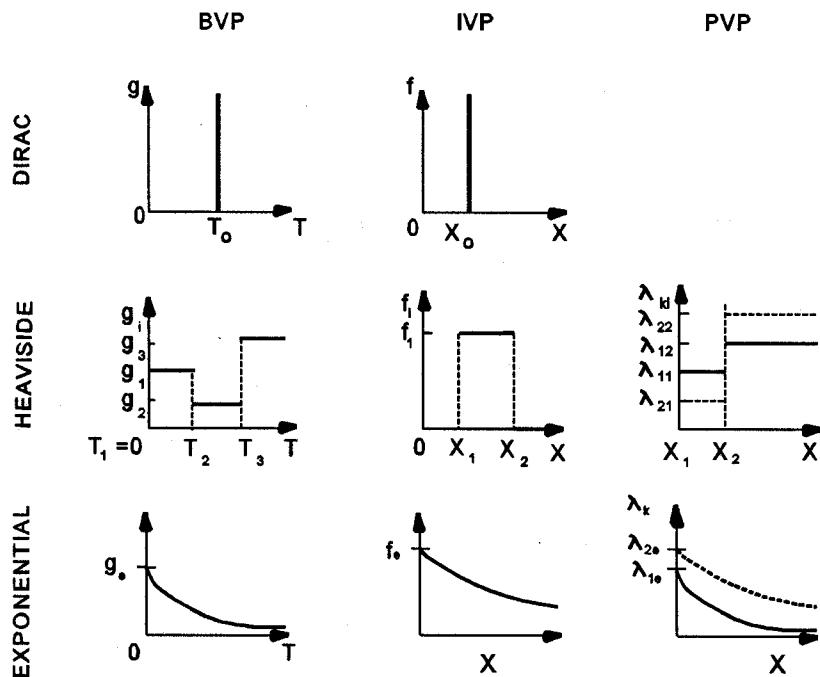


Fig. 1. Schematic of Dirac, Heaviside, and exponential functions to describe solute input versus time for the BVP, the initial concentration versus depth for the IVP, and the production profile for the equilibrium (solid line) and nonequilibrium (dashed line) phases for the PVP.

We will further illustrate the specification of mathematical conditions over different regions for the example of an initial value problem (IVP) where all subfunctions (i.e., f_x, f_y and $f_z; f_{xy}, f_{yz}$, and f_{xz}) are given by Heaviside functions. The following regions were considered: (a) semi-infinite rectangular, (b) finite rectangular, (c) cylindrical, and (d) spherical. The solute is initially contained in two regions — each with a different, uniform initial concentration. Appendix C gives the instructions to prepare the input file for solving these types of problems with N3DADE.

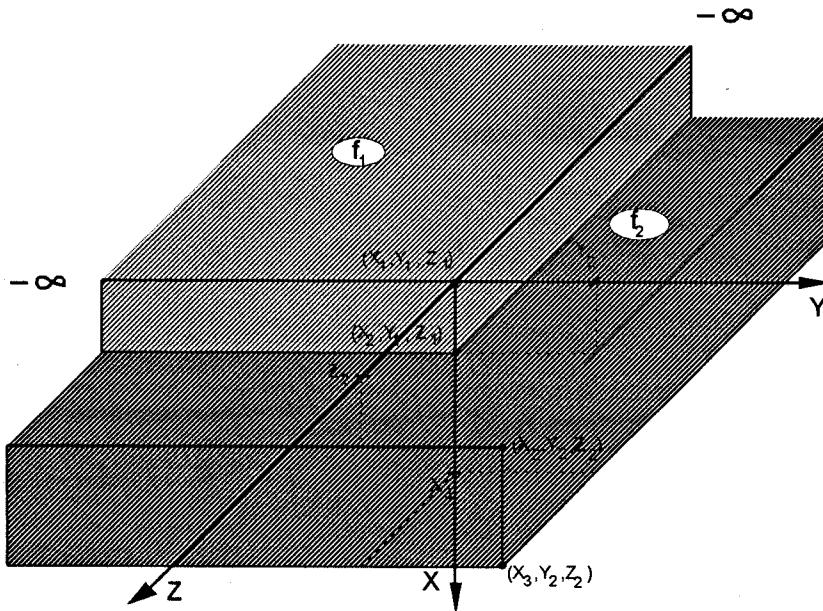


Fig. 2. Initial condition prescribed over semi-infinite rectangles in the transverse plane.

For the two semi-infinite slabs shown in Fig. 2, the initial condition is given by

$$f(X, Y, Z) = \begin{cases} f_1 & X_1 < X < X_2 \quad -\infty < Y < Y_1 \quad -\infty < Z < Z_1 \\ f_2 & X_2 < X < X_3 \quad -\infty < Y < Y_2 \quad -\infty < Z < Z_2 \\ 0 & \text{otherwise} \end{cases} \quad (76)$$

In this case the upper corner of the first slab coincides with the origin of the Cartesian coordinate system ($X_1=Y_1=Z_1=0$). The initial concentration in the layer between $X_1=0$ and X_2 is equal to f_1 in the semi-infinite transverse plane given by $Y < Y_1$ and $Z < Z_1$ and equal to zero elsewhere; similarly the concentration between X_2 and X_3 is equal to f_2 in the semi-infinite rectangle given by $Y < Y_2$ and $Z < Z_2$ and zero elsewhere.

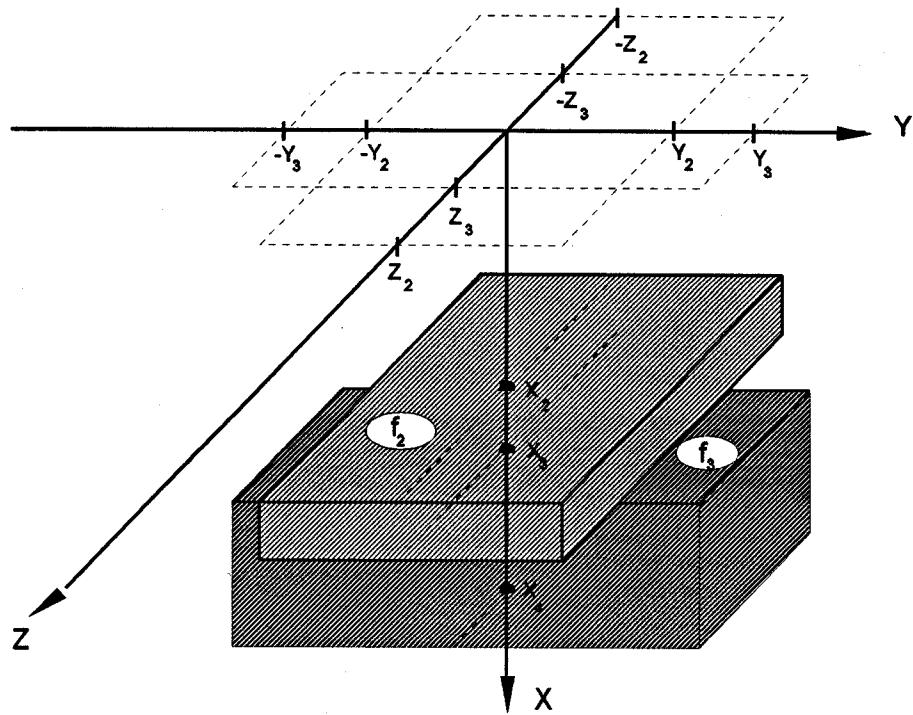


Fig. 3. Initial condition prescribed over finite rectangles in the transverse plane.

Figure 3 shows two rectangular parallelepipeds for solute initially present in layers bounded by a finite transverse rectangle according to the condition

$$f(X, Y, Z) = \begin{cases} f_2 & X_2 < X < X_3 \quad -Y_2 < Y < Y_2 \quad -Z_2 < Z < Z_2 \\ f_3 & X_3 < X < X_4 \quad -Y_3 < Y < Y_3 \quad -Z_3 < Z < Z_3 \\ 0 & \text{otherwise} \end{cases} \quad (77)$$

There is no solute between $X_1=0$ and X_2 ; the initial concentration in the layer $X_2 < X < X_3$ is equal to f_2 in a finite region of the transverse plane given by $|Y| < Y_2$ and $|Z| < Z_2$, and equal to zero elsewhere. The concentration in the parallelepiped with coordinates $(X_3, \pm Y_3, \pm Z_3)$ and $(X_4, \pm Y_3, \pm Z_3)$ is equal to f_3 .

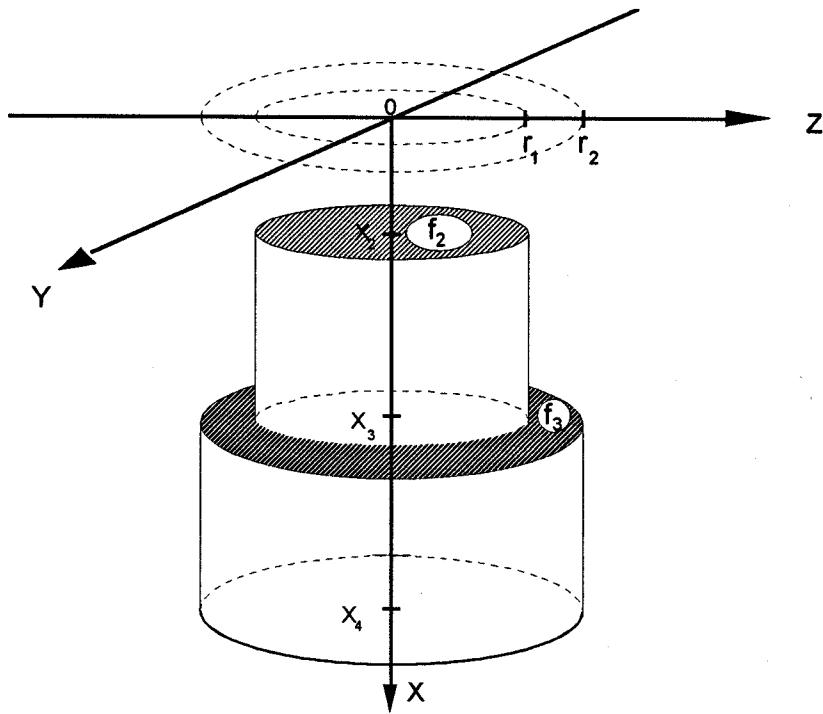


Fig. 4. Initial condition prescribed over circular regions in the transverse plane.

Figure 4 displays an example where the solute is initially confined to cylindrical regions. The initial profile is defined as follows

$$f(X, Y, Z) = \begin{cases} f_2 & X_2 < X < X_3 \quad r_c = \sqrt{Y^2 + Z^2} < r_1 \\ f_3 & X_3 < X < X_4 \quad r_c = \sqrt{Y^2 + Z^2} < r_2 \\ 0 & \text{otherwise} \end{cases} \quad (78)$$

The concentration at $T=0$ is equal to f_2 between X_2 and X_3 in a hypothetical cylinder with radius r_1 ; the initial concentration is equal to f_3 between X_3 and X_4 when the distance perpendicular to the X -coordinate is less than r_2 , and is equal to zero everywhere else.

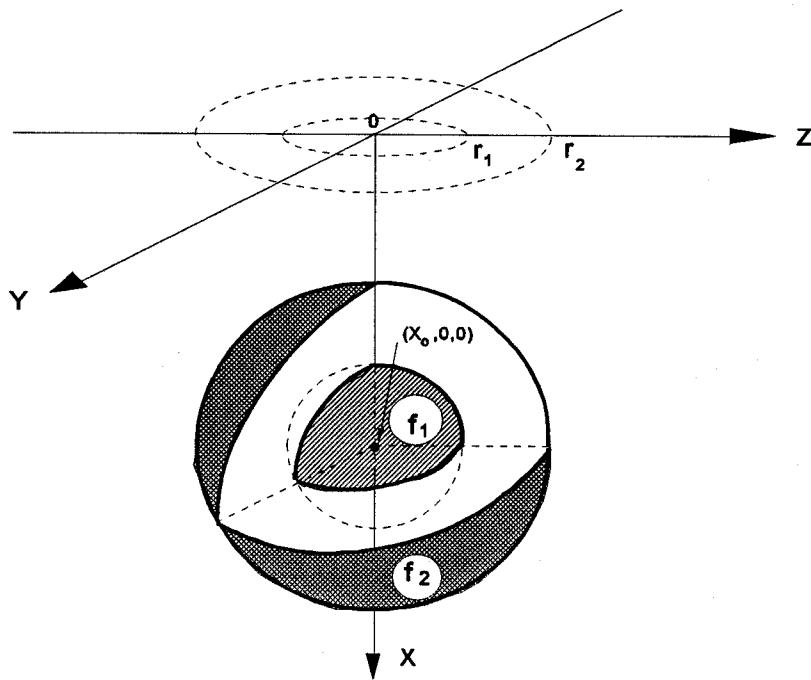


Fig. 5. Initial condition prescribed over spherical regions.

Figure 5 shows a composite sphere, with center $(X_0, 0, 0)$, to depict the initial condition:

$$f(X, Y, Z) = \begin{cases} f_1 & r_s = \sqrt{(X-X_0)^2 + Y^2 + Z^2} < r_1 \\ f_2 & r_1 < r_s = \sqrt{(X-X_0)^2 + Y^2 + Z^2} < r_2 \\ 0 & \text{otherwise} \end{cases} \quad (79)$$

The initial concentration is equal to f_1 in the inner sphere, with radius r_1 , while the concentration in the outer shell, between radial distances r_1 and r_2 , is equal to f_2 . The concentration outside the sphere with radius r_2 is equal to zero.

3.2. Derivation of Specific Solutions

The longitudinal conditions and derive the corresponding expressions for the equilibrium and nonequilibrium concentrations are derived in sections 3.2.1 through 3.2.3. The solutions contain generic terms for the transverse part of the solutions. The options for the transverse distributions and the resulting expressions for the transverse part of the solution are provided in section 3.2.4. Again, if more than one boundary, initial or production process occurs; the overall solution may be obtained by simply adding the solutions for the different subproblems since the transport problem is linear.

3.2.1. Boundary Value Problem

The *Dirac* function is used to describe instantaneous application of a finite amount of mass according to:

$$g_T(T) = M \delta(T-T_0) \quad (80)$$

Note that M is the solute mass applied per unit area of the liquid phase; this amount is normalized through division by the product Lc_o . The equilibrium solution is readily obtained from (44):

$$\begin{aligned} C_1(X, Y, Z, T) &= M \left[\exp\left(-\frac{\alpha(T-T_0)}{\beta R}\right) \Gamma_Y(Y, T-T_0) \Gamma_Z(Z, T-T_0) G(X, T-T_0) \right. \\ &\quad \left. + \int_0^{T-T_0} \sqrt{\frac{\alpha_2 \tau}{T-T_0 - \tau}} H_1(\tau, T-T_0) \Gamma_Y(Y, \tau) \Gamma_Z(Z, \tau) G(X, \tau) d\tau \right] \end{aligned} \quad (81)$$

The functions Γ_Y and Γ_Z represent a generic transverse part of the solution (cf. (43)), which will be further specified in section 3.2.4. The integrals in the nonequilibrium solution (45) are rearranged using Fubini's theorem to obtain:

$$C_2(X, Y, Z, T) = \frac{\alpha M}{(1-\beta)R} \int_0^{T-T_0} H_0(\tau, T-T_0) \Gamma_Y(Y, \tau) \Gamma_Z(Z, \tau) G(X, \tau) d\tau \quad (82)$$

The *Heaviside* function for the boundary value problem is given by

$$g_i(T) = g_i [U(T-T_i) - U(T-T_{i+1})] \quad (i = 1, 2, \dots) \quad (83)$$

where U is a Heaviside unit-step function to denote application of a solution with concentration g_i between times T_i and T_{i+1} . Substitution of this condition into (44) and subsequent application of Fubini's theorem and Eq.(64) yields a relatively simple solution in terms of Goldstein's J -function:

$$C_1(X, Y, Z, T) = g_i \int_{T-T_{i+1}}^{T-T_i} \exp\left(-\frac{\omega\mu_2\tau}{(\omega+\mu_2)\beta R}\right) J(p, q) \Gamma_Y(Y, \tau) \Gamma_Z(Z, \tau) G(X, \tau) d\tau \quad (84)$$

The nonequilibrium concentration is obtained by using Eq.(45) and Fubini's theorem. With help of the identity

$$\int_{\eta}^T \exp\left(-\frac{\omega+\mu_2}{(1-\beta)R}(T-\tau)\right) J(p', q') d\tau = \frac{(1-\beta)R}{\omega+\mu_2} [1 - J(q, p)] \quad (85)$$

we can establish that

$$C_2(X, Y, Z, T) = \frac{\omega g_i}{\omega+\mu_2} \int_{T-T_{i+1}}^{T-T_i} \exp\left(-\frac{\omega\mu_2\tau}{(\omega+\mu_2)\beta R}\right) [1 - J(q, p)] \Gamma_Y(Y, \tau) \Gamma_Z(Z, \tau) G(X, \tau) d\tau \quad (86)$$

The third specific case involves an input function which decreases *exponentially* with time according to

$$g(T) = g_e \exp(-\alpha T) \quad (87)$$

The equilibrium concentration can be rewritten as

$$\begin{aligned} C_1(X, Y, Z, T) &= g_e \int_0^T \exp\left(-\alpha(T-\tau) - \frac{\omega\tau}{\beta R}\right) \Gamma_Y(Y, \tau) \Gamma_Z(Z, \tau) G(X, \tau) d\tau \\ &\quad + g_e \int_0^T \int_{\eta}^T \sqrt{\frac{a_2\eta}{\tau-\eta}} I_1[2\sqrt{a_2(\tau-\eta)}\eta] \\ &\quad \times \exp\left[-\alpha(T-\tau) - \frac{\omega\eta}{\beta R} - \frac{\omega+\mu_2}{(1-\beta)R}(\tau-\eta)\right] \Gamma_Y(Y, \eta) \Gamma_Z(Z, \eta) G(X, \eta) d\tau d\eta \end{aligned} \quad (88)$$

Integration by parts leads to

$$\begin{aligned} \int_{\eta}^T \exp(w\tau) \sqrt{\frac{a_2\eta}{\tau-\eta}} I_1[2\sqrt{a_2(\tau-\eta)}\eta] d\tau &= \exp(w\tau) I_0[2\sqrt{a_2(\tau-\eta)}\eta] \Big|_{\eta}^T \\ &\quad - \int_{\eta}^T w \exp(w\tau) I_0[2\sqrt{a_2(\tau-\eta)}\eta] d\tau \quad , \quad w = \alpha - \frac{\omega+\mu_2}{(1-\beta)R} \end{aligned} \quad (89a,b)$$

No closed-form expression likely exist for the integration of the product of an exponential function

and a zero-order modified Bessel function [Luke, 1962]. After expressing I_0 as [cf. 9.6.12 of Olver, 1965]

$$I_0[\sqrt{a_2\tau\eta}] = 1 + \frac{a_2\eta}{(1!)^2} \tau + \frac{(a_2\eta)^2}{(2!)^2} \tau^2 + \frac{(a_2\eta)^3}{(3!)^2} \tau^3 + \dots \quad (90)$$

we can carry out the following integration [cf. 2.321.2 of Gradshteyn and Ryzhik, 1980]:

$$\begin{aligned} \int_{\eta}^T \exp(w\tau) I_0[2\sqrt{a_2(\tau-\eta)\eta}] d\tau &= \\ \frac{1}{w} \exp(wT) \{ I_0[2\sqrt{a_2(T-\eta)\eta}] + \Phi_1(\eta) \} - \frac{1}{w} \exp[(w - \frac{a_2}{w})\eta] \end{aligned} \quad (91)$$

$$\Phi_1(\eta) = \sum_{n=1}^{\infty} \sum_{k=1}^n \frac{(-1)^k}{w^k} \frac{(a_2\eta)^n}{n!} \frac{(T-\eta)^{n-k}}{(n-k)!} \quad (92)$$

The equilibrium concentration may then be given as

$$\begin{aligned} C_1(X, Y, Z, T) &= g_e \int_0^T \exp\left[-\alpha(T-\tau) - \frac{\omega\tau}{\beta R}\right] \\ &\times \left\{ \exp\left(-\frac{a_2\tau}{w}\right) - \exp[w(T-\tau)] \Phi_1(\tau) \right\} \Gamma_Y(Y, \tau) \Gamma_Z(Z, \tau) G(X, \tau) d\tau \end{aligned} \quad (93)$$

In most cases a convergent solution will be obtained when n is at most 25. The solution will become more difficult to evaluate accurately for relatively large values for a , w , and T . Similar problems have been reported by Lassey [1982] for the series approximation of the J -function as used by De Smedt and Wierenga [1979b].

The nonequilibrium solution is obtained with the help of Eq.(45) to give

$$\begin{aligned} C_2(X, Y, Z, T) &= \frac{\omega g_e}{(1-\beta)R} \int_0^T \exp\left[-\frac{\omega\tau}{\beta R} - \frac{\omega+\mu_2}{(1-\beta)R}(T-\tau)\right] \\ &\left[\frac{1}{w} \exp\left(-\frac{a_2\tau}{w}\right) \{ 1 - \exp[-w(T-\tau)] \} - \Phi_2(\tau) \right] \Gamma(Y, \tau) \Gamma(Z, \tau) G(X, \tau) d\tau \end{aligned} \quad (94)$$

where

$$\Phi_2(\tau) = \sum_{n=1}^{\infty} \sum_{k=1}^n \frac{(-1)^k}{w^k} \frac{(a_2\tau)^n}{n!} \frac{(T-\tau)^{n-k+1}}{(n-k+1)(n-k)!} \quad (95)$$

3.2.2. Initial Value Problem

We will first list the conditions and solutions for a Dirac, Heaviside, or exponential initial profile; these solutions can be used in combination with one or two transversal distributions for circular or rectangular regions. At the end of this section we treat the conditions and solutions for a Heaviside or exponential distribution for spherical regions.

Instantaneous release of a normalized mass of solute at location X_0 for an arbitrary initial time can be described with a *Dirac* function according to:

$$f(X) = M\delta(X-X_0) \quad (96)$$

The solutions can be readily obtained from the general solution given by Eqs. (53) and (54):

$$\begin{aligned} C_1(X,Y,Z,T) &= M \left[\exp\left(-\frac{\omega T}{\beta R}\right) \Gamma_Y(Y,T) \Gamma_Z(Z,T) G(X_0,T;X) \right. \\ &\quad \left. + \int_0^T \left(\frac{\omega}{\beta R} H_0(\tau,T) + \sqrt{\frac{a_2 \tau}{T-\tau}} H_1(\tau,T) \right) \Gamma_Y(Y,\tau) \Gamma_Z(Z,\tau) G(X_0,\tau;X) d\tau \right] \end{aligned} \quad (97)$$

$$C_2(X,Y,Z,T) = \frac{\omega M}{(1-\beta)R} \int_0^T \left(H_0(\tau,T) + \sqrt{\frac{(1-\beta)(T-\tau)}{\beta\tau}} H_1(\tau,T) \right) \Gamma_Y(Y,\tau) \Gamma_Z(Z,\tau) G(X_0,\tau;X) d\tau \quad (98)$$

Note that the term containing the initial condition has been omitted from the nonequilibrium solution because it pertains to an infinitely small region at X_0 .

The *Heaviside* initial profile is given by

$$f_X(X) = f_i [U(X-X_i) - U(X-X_{i+1})] \quad (i = 1, 2, \dots) \quad (99)$$

The equilibrium solution is obtained by substituting this condition into (53) and evaluating the following integral using a table of Laplace transforms:

$$\int_{X_1}^{X_2} G(\xi, \tau, X) d\xi = -G_1(X, \tau, \xi) \Big|_{\xi=X_1}^{\xi=X_2} \quad (100)$$

The equilibrium solution can be written as

$$\begin{aligned} C_1(X,Y,Z,T) &= f_i \exp\left(-\frac{\omega T}{\beta R}\right) [G_1(X,T;X_i) - G_1(X,T;X_{i+1})] \Gamma_Y(Y,T) \Gamma_Z(Z,T) \\ &\quad + f_i \int_0^T \left(\frac{\omega}{\beta R} H_0(\tau,T) + \sqrt{\frac{a_2 \tau}{T-\tau}} H_1(\tau,T) \right) [G_1(X,\tau;X_i) - G_1(X,\tau;X_{i+1})] \Gamma_Y(Y,\tau) \Gamma_Z(Z,\tau) d\tau \end{aligned} \quad (101)$$

where the expressions for G_1 can be found in Table 2. Similarly, the nonequilibrium solution is

$$C_2(X, Y, Z, T) = f_Y(Y)f_Z(Z)f_i[U(X-X_i) - U(X-X_{i+1})] \exp\left(-\frac{\omega+\mu_2}{(1-\beta)R}T\right) + \frac{\omega f_i}{(1-\beta)R} \int_0^T \left(H_0(\tau, T) + \sqrt{\frac{(1-\beta)(T-\tau)}{\beta\tau}} H_1(\tau, T) \right) \times [G_1(X, \tau, X_i) - G_1(X, \tau, X_{i+1})] \Gamma_Y(Y, \tau) \Gamma_Z(Z, \tau) d\tau \quad (102)$$

An initial profile that decreases *exponentially* with depth is given as

$$f(X) = f_e \exp(-\alpha X) \quad (103)$$

The solution for this problem utilizes the following integral:

$$\int_0^\infty \exp(-\alpha\xi) G(\xi, \tau, X) d\xi = G_2(X, \tau, \alpha) \quad (104)$$

The equilibrium concentration for the exponential profile is

$$C_1(X, Y, Z, T) = f_Y(Y)f_Z(Z)f_e \exp\left(-\frac{\omega T}{\beta R}\right) G_2(X, T, \alpha) + f_e \int_0^T \left(\frac{\omega}{\beta R} H_0(\tau, T) + \sqrt{\frac{a_2 \tau}{T-\tau}} H_1(\tau, T) \right) \Gamma_Y(Y, \tau) \Gamma_Z(Z, \tau) G_2(X, \tau, \alpha) d\tau \quad (105)$$

whereas the nonequilibrium concentration is given by

$$C_2(X, Y, Z, T) = f_Y(Y)f_Z(Z)f_e \exp\left(-\alpha X - \frac{\omega+\mu_2}{(1-\beta)R}T\right) + \frac{\omega f_e}{(1-\beta)R} \int_0^T \left(H_0(\tau, T) + \sqrt{\frac{(1-\beta)(T-\tau)}{\beta\tau}} H_1(\tau, T) \right) \Gamma_Y(Y, \tau) \Gamma_Z(Z, \tau) G_2(X, \tau) d\tau \quad (106)$$

Spherical Regions. The *Heaviside* function for a step change in initial concentration for a spherical region is given by

$$f_X(X)f_Y(Y)f_Z(Z) = f_i[U(r_s - r_{i-1}) - U(r_s - r_i)] = \begin{cases} f_i & r_{i-1} < r_s = \sqrt{(X-X_0)^2 + Y^2 + Z^2} < r_i \\ 0 & \text{otherwise} \end{cases} \quad (107)$$

The solutions for the equilibrium and nonequilibrium concentration are obtained by formulating the appropriate limits of integration in the general solution, and evaluating the integral with respect to dummy variable ξ in (53) and (54). The following expressions were obtained

$$C_1(X, Y, Z, T) = f_i \exp\left(-\frac{\omega T}{\beta R}\right) \left(\int_{X_0 - r_i}^{X_0 + r_i} \Gamma_6(\xi, Y, Z, T; r_i) G(\xi, T; X) d\xi \right. \\ \left. - \int_{X_0 - r_{i-1}}^{X_0 + r_{i-1}} \Gamma_6(\xi, Y, Z, T; r_{i-1}) G(\xi, T; X) d\xi \right) + f_i \int_0^T \left(\frac{\omega}{\beta R} H_0(\tau, T) + \sqrt{\frac{a_2 \tau}{T-\tau}} H_1(\tau, T) \right) \\ \times \left(\int_{X_0 - r_i}^{X_0 + r_i} \Gamma_6(\xi, Y, Z, \tau; r_i) G(\xi, \tau; X) d\xi - \int_{X_0 - r_{i-1}}^{X_0 + r_{i-1}} \Gamma_6(\xi, Y, Z, \tau; r_{i-1}) G(\xi, \tau; X) d\xi \right) d\tau \quad (108)$$

$$C_2(X, Y, Z, T) = f_i [U(r_s - r_{i-1}) - U(r_s - r_i)] \exp\left(-\frac{\omega + \mu_2}{(1-\beta)R} T\right) \\ + \frac{\omega f_i}{(1-\beta)R} \int_0^T \left(\int_{X_0 - r_i}^{X_0 + r_i} \Gamma_6(\xi, Y, Z, \tau; r_i) G(\xi, \tau; X) d\xi - \int_{X_0 - r_{i-1}}^{X_0 + r_{i-1}} \Gamma_6(\xi, Y, Z, \tau; r_{i-1}) G(\xi, \tau; X) d\xi \right) d\tau \quad (109)$$

If the initial concentration decreases *exponentially* from the centroid $(X_0, 0, 0)$, we have:

$$f_X(X)f_Y(Y)f_Z(Z) = f_e \exp\left(-\alpha \sqrt{(X-X_0)^2 + Y^2 + Z^2}\right) \quad (110)$$

Expressions for the equilibrium and nonequilibrium concentrations follow directly from substituting this condition in the general solution

$$C_1(X, Y, Z, T) = f_e \int_0^\infty \left[\exp\left(-\frac{\omega T}{\beta R}\right) \Gamma_7(\xi, Y, T) G(\xi, T; X) \right. \\ \left. + \int_0^T \left(\frac{\omega}{\beta R} H_0(\tau, T) + \sqrt{\frac{a_2 \tau}{T-\tau}} H_1(\tau, T) \right) \Gamma_7(\xi, Y, \tau) G(\xi, \tau; X) d\tau \right] d\xi \quad (111)$$

$$C_2(X, Y, Z, T) = f_e \exp\left[-\alpha \sqrt{(X-X_0)^2 + Y^2 + Z^2} - \frac{\omega + \mu_2}{(1-\beta)R} T\right] \\ + \frac{\omega f_e}{(1-\beta)R} \int_0^\infty \int_0^T \left(H_0(\tau, T) + \sqrt{\frac{(1-\beta)(T-\tau)}{\beta \tau}} H_1(\tau, T) \right) \Gamma_7(\xi, Y, \tau) G(\xi, \tau; X) d\tau d\xi \quad (112)$$

3.2.3. Production Value Problem

Solutions for problems involving specific production profiles can be readily obtained using the above results for the initial value problem. We will omit the Dirac function since this distribution is not very realistic for solute production. The *Heaviside* production profile is given by

$$\lambda_{kX}(X) = \lambda_{ki} [U(X-X_i) - U(X-X_{i+1})] \quad (k=1,2) \quad (113)$$

The specific solutions for this production pulse are

$$C_1(X, Y, Z, T) = \frac{1}{\beta R} \int_0^T \exp\left(-\frac{\omega\mu_2\tau}{(\omega+\mu_2)\beta R}\right) \left(\lambda_{1i} J(p, q) + \frac{\omega\lambda_{2i}}{\omega+\mu_2} [1-J(q, p)] \right) \\ \times [G_1(X, \tau, X_i) - G_1(X, \tau, X_{i+1})] \Gamma_Y(Y, \tau) \Gamma_Z(Z, \tau) d\tau \quad (114)$$

$$C_2(X, Y, Z, T) = \frac{\lambda_{2Y}(Y) \lambda_{2Z}(Z) \lambda_{2i} [U(X-X_i) - U(X-X_{i+1})]}{\omega+\mu_2} \left[1 - \exp\left(-\frac{\omega+\mu_2}{(1-\beta)R} T\right) \right] \\ + \frac{\omega}{\beta R (\omega+\mu_2)} \int_0^T \exp\left(-\frac{\omega\mu_2\tau}{(\omega+\mu_2)\beta R}\right) [G_1(X, \tau, X_i) - G_1(X, \tau, X_{i+1})] \Gamma_Y(Y, \tau) \Gamma_Z(Z, \tau) \\ \times \left\{ \lambda_{1i} [J(q, p) - \exp(-p-q) I_0(2\sqrt{pq})] + \frac{\omega\lambda_{2i}}{\omega+\mu_2} \left[1 - J(q, p) + \sqrt{\frac{q}{p}} \exp(-p-q) I_1(2\sqrt{pq}) \right] \right\} d\tau \quad (115)$$

The resident and flux type expressions for G_1 are given in Table 2 whereas Γ_Y and Γ_Z are to be specified in section 3.2.4.

Zero-order solute production profiles that decrease *exponentially* with depth are given by

$$\lambda_k(X) = \lambda_{ke} \exp(-\alpha X) \quad (k=1,2) \quad (116)$$

The solutions for the exponential production profile follow from the general solutions in a similar manner as for the IVP. The resulting expressions are

$$C_1(X, Y, Z, T) = \frac{1}{\beta R} \int_0^T \exp\left(-\frac{\omega\mu_2\tau}{(\omega+\mu_2)\beta R}\right) \\ \times \left(\lambda_{1e} J(p, q) + \frac{\omega\lambda_{2e}}{\omega+\mu_2} [1 - J(q, p)] \right) \Gamma_Y(Y, \tau) \Gamma_Z(Z, \tau) G_2(X, \tau, \alpha) d\tau \quad (117)$$

$$\begin{aligned}
C_2(X, Y, Z, T) = & \frac{\lambda_{2Y}(Y) \lambda_{2Z}(Z) \lambda_{2e} \exp(-\alpha X)}{\omega + \mu_2} \left[1 - \exp \left(-\frac{\omega + \mu_2}{(1-\beta)R} T \right) \right] \\
& + \frac{\omega}{\beta R (\omega + \mu_2)} \int_0^T \exp \left(-\frac{\omega \mu_2 \tau}{(\omega + \mu_2) \beta R} \right) \left\{ \lambda_{1e} [J(q, p) - \exp(-p-q) I_0(2\sqrt{pq})] \right. \\
& \left. + \frac{\omega \lambda_{2e}}{\omega + \mu_2} \left[1 - J(q, p) + \sqrt{\frac{q}{p}} \exp(-p-q) I_1(2\sqrt{pq}) \right] \right\} \Gamma_Y(Y, \tau) \Gamma_Z(Z, \tau) G_2(X, \tau, \alpha) d\tau
\end{aligned} \tag{118}$$

where, as noted, G_2 is defined in Table 2.

Spherical Regions. The *Heaviside* function for a production pulse along a (hypothetical) spherical coordinate is given by:

$$\lambda_{kX}(X) \lambda_{kY}(Y) \lambda_{kZ}(Z) = \begin{cases} \lambda_{ki} & r_{i-1} < \sqrt{(X-X_0)^2 + Y^2 + Z^2} < r_i \\ 0 & \text{otherwise} \end{cases} \tag{119}$$

The equilibrium and nonequilibrium concentration for this type of PVP are

$$\begin{aligned}
C_1(X, Y, Z, T) = & \frac{1}{\beta R} \int_0^T \exp \left(-\frac{\omega \mu_2 \tau}{(\omega + \mu_2) \beta R} \right) \left(\lambda_{1i} J(p, q) + \frac{\omega \lambda_{2i}}{\omega + \mu_2} [1 - J(q, p)] \right) \\
& \left(\int_{X_0 - r_i}^{X_0 + r_i} \Gamma_6(Y, Z, \tau, r_i) G(\xi, \tau, X) d\xi - \int_{X_0 - r_{i-1}}^{X_0 + r_{i-1}} \Gamma_6(Y, Z, \tau, r_{i-1}) G(\xi, \tau, X) d\xi \right) d\tau
\end{aligned} \tag{120}$$

$$\begin{aligned}
C_2(X, Y, Z, T) = & \frac{\lambda_{2i}}{\omega + \mu_2} [U(r_s - r_{i-1}) - U(r_s - r_i)] \left[1 - \exp \left(-\frac{\omega + \mu_2}{(1-\beta)R} T \right) \right] \\
& + \frac{\omega}{\beta R (\omega + \mu_2)} \int_0^T \exp \left(-\frac{\omega \mu_2 \tau}{(\omega + \mu_2) \beta R} \right) \left\{ \lambda_{1i} [J(q, p) - \exp(-p-q) I_0(2\sqrt{pq})] \right. \\
& \left. + \frac{\omega \lambda_{2i}}{\omega + \mu_2} \left[1 - J(q, p) + \sqrt{\frac{q}{p}} \exp(-p-q) I_1(2\sqrt{pq}) \right] \right\} \\
& \times \left(\int_{X_0 - r_i}^{X_0 + r_i} \Gamma_6(\xi, Y, Z, \tau, r_i) G(\xi, \tau, X) d\xi - \int_{X_0 - r_{i-1}}^{X_0 + r_{i-1}} \Gamma_6(\xi, Y, Z, \tau, r_{i-1}) G(\xi, \tau, X) d\xi \right) d\tau
\end{aligned} \tag{121}$$

For a zero-order production process that decreases *exponentially* with distance from $(X_0, 0, 0)$, the production profile may be specified as:

$$\lambda_{kX}(X)\lambda_{kY}(Y)\lambda_{kZ}(Z) = \lambda_{ke} \exp\left(-\alpha\sqrt{(X-X_0)^2 + Y^2 + Z^2}\right) \quad (122)$$

The corresponding equilibrium and nonequilibrium concentrations are

$$C_1(X, Y, Z, T) = \frac{1}{\beta R} \int_0^T \exp\left(-\frac{\omega\mu_2\tau}{(\omega+\mu_2)\beta R}\right) \times \left(\lambda_{1e} J(p, q) + \frac{\omega}{\omega+\mu_2} \lambda_{2e} [1 - J(q, p)] \right) \int_0^\infty \Gamma_7(\xi, Y, Z, \tau) G(\xi, \tau, X) d\xi d\tau \quad (123)$$

$$C_2(X, Y, Z, T) = \frac{\lambda_2}{\omega+\mu_2} \exp\left[-\alpha\sqrt{(X-X_0)^2 + Y^2 + Z^2}\right] \left[1 - \exp\left(-\frac{\omega+\mu_2}{(1-\beta)R} T\right) \right] + \frac{\omega}{\beta R (\omega+\mu_2)} \int_0^T \exp\left(-\frac{\omega\mu_2\tau}{(\omega+\mu_2)\beta R}\right) \left\{ \lambda_{1e} [J(q, p) - \exp(-p-q) I_0(2\sqrt{pq})] \right. \\ \left. + \frac{\omega\lambda_{2e}}{\omega+\mu_2} \left[1 - J(q, p) + \sqrt{\frac{q}{p} \exp(-p-q) I_1(2\sqrt{pq})} \right] \right\} \int_0^\infty \Gamma_7(\xi, Y, Z, T) G(\xi, \tau, X) d\xi d\tau \quad (124)$$

3.2.4. Transversal Solutions

The solution for the transverse direction still needs to be specified. We may select either a Dirac, Heaviside, or exponential function for a rectangular geometry; these functions should be specified for both the Y and the Z direction. The program can evaluate problems involving circular regions, in which case a Heaviside or exponential function may be selected for the (radial) direction. No transversal distribution should be specified in case of a spherical geometry. In this section we will first consider the rectangular geometry. We will state possible functions for the Y -direction and integrate the product of the transverse condition and the auxiliary function $\Gamma(\varphi, Q, \tau)$ to obtain specific expressions for Γ as listed in Table 3. The same information for the Z -coordinate can be readily inferred. Next, the transversal distribution will be specified for a circular geometry using a radial coordinate as dependent variable.

Rectangular Regions. The *Dirac* function for an exclusive nonzero condition in the Y -direction about Y_0 is:

$$\left. \begin{array}{l} g_Y(Y) \\ f_Y(Y) \\ \lambda_{kY}(Y) \end{array} \right\} = \delta(Y - Y_0) \quad (125)$$

The transverse integration in the general solutions can be readily carried out. The result is

$$\int_{-\infty}^{\infty} \delta(Y - \varphi - Y_0) \Gamma_Y(\varphi, T) d\varphi = \Gamma_1(Y - Y_0, T) \quad (126)$$

where the expression for Γ_1 is given in Table 3. This table contains expressions resulting from integrating the transverse auxiliary functions for different distributions.

A step change in the input, initial, or production condition in the transverse direction is represented with a *Heaviside* function. A pulse between two arbitrary positions Y_i and Y_{i+1} is described with Heaviside functions according to

$$\left. \begin{array}{l} g_Y(Y) \\ f_Y(Y) \\ \lambda_{kY}(Y) \end{array} \right\} = U(Y - Y_i) - U(Y - Y_{i+1}) = \begin{cases} 1 & Y_i < Y < Y_{i+1} \\ 0 & \text{otherwise} \end{cases} \quad (127)$$

Integration of the Y -dependent part of the general solutions now yields

$$\int_{-\infty}^{\infty} [U(Y - \varphi - Y_i) - U(Y - \varphi - Y_{i+1})] \Gamma_Y(\varphi, T) d\varphi = \Gamma_2(Y, T; Y_{i+1}) - \Gamma_2(Y, T; Y_i) \quad (128)$$

For an *exponential* profile, with plane of symmetry given by the coordinates (X, Y_0, Z) , the input, initial or production profile is defined as

$$\left. \begin{array}{l} g_Y(Y) \\ f_Y(Y) \\ \lambda_{kY}(Y) \end{array} \right\} = \exp(-\alpha|Y - Y_0|) \quad (129)$$

Substituting this condition in the general solutions for the BVP, IVP, or PVP, and integrating with respect to the dummy variable φ , yields the following result:

$$\int_{-\infty}^{\infty} \exp(-\alpha|Y - \varphi - Y_0|) \Gamma_Y(\varphi, T) d\varphi = \Gamma_3(Y, T; Y_0) \quad (130)$$

Circular Regions. Conditions may be specified over circular regions by combining terms for the Y and Z coordinates. Transverse distributions with a circular pattern arise for the BVP if the concentration of the influent has an arbitrary point of symmetry at the surface (i.e., the YZ plane at $X=0$) and, similarly, for the IVP or PVP if the initial or production profiles have the X coordinate as line of symmetry. Note that there is no reason to specify a Dirac condition over a circular region.

A Heaviside profile may be given as

$$\left. \begin{array}{l} g_Y(Y) g_Z(Z) \\ f_Y(Y) g_Z(Z) \\ \lambda_{kY}(Y) \lambda_{kZ}(Z) \end{array} \right\} = U(r_c - r_i) - U(r_c - r_{i+1}) , \quad r_c = \sqrt{Y^2 + Z^2} \quad (131a,b)$$

The double integral in the general solution can be simplified by integrating with respect to Z :

$$\begin{aligned} & \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \{ U[\sqrt{(Y-\varphi)^2 + (Z-\Omega)^2} - r_i] - U[\sqrt{(Y-\varphi)^2 + (Z-\Omega)^2} - r_{i+1}] \} \Gamma_Y(\varphi, T) \Gamma_Z(\Omega, T) d\Omega d\varphi \\ &= \Gamma_4(Y, Z, T; r_{i+1}) - \Gamma_4(Y, Z, T; r_i) \end{aligned} \quad (132)$$

An exponential profile with the axis of symmetry at $(X, 0, 0)$ is given by

$$\left. \begin{array}{l} g_Y(Y) g_Z(Z) \\ f_Y(Y) f_Z(Z) \\ \lambda_{kY}(Y) \lambda_{kZ}(Z) \end{array} \right\} = \exp(-\alpha r_c) \quad (133)$$

No analytical integration of the transverse expression in the general solution is now apparent.

3.3. Summary of Conditions

Table 4 summarizes the different combinations of longitudinal and transversal profiles for which N3DADE evaluates the equilibrium and nonequilibrium solutions. The upper part of the Table deals with a rectangular geometry; combinations for some circular and a few spherical geometries are listed in the lower part of the table. The first column of Table 4 numbers the different problems, this number is the same as the parameter NP in the input file. The second column identifies the combination of transverse functions for each number; no transverse functions are involved for a spherical initial or production function. The right-hand side of the table specifies the longitudinal function for each problem number as illustrated in Fig. 1; Dirac (D), Heaviside (H), or exponential (E) functions. The mode of the problem, MP, needs to be specified to determine whether the combination applies to a boundary value problem (BVP), initial value problem (IVP), and production value problem (PVP).

Table 4. Combinations of Dirac (D), Heaviside (H), and Exponential (E) Functions
for Specifying the Mathematical Conditions of the BVP, IVP, or PVP†

NP ‡	$\Gamma_1(Y, T)$ $\Gamma_2(Z, T)$	BVP	IVP	PVP
<i>Rectangular Geometry</i>				
1	$\Gamma_1(Y-Y_0, T) \Gamma_1(Z-Z_0, T)$	D D D	D D D	- - -
2	$\Gamma_1(Y-Y_0, T)[\Gamma_2(Z, T; Z_{i+1})-\Gamma_2(Z, T; Z_i)]$	D D H	D D H	- - -
3	$\Gamma_1(Y-Y_0, T)\Gamma_3(Z, T; Z_0)$	D D E	D D E	- - -
4	$[\Gamma_2(Y, T; Y_{i+1})-\Gamma_2(Y, T; Y_i)]\Gamma_1(Z-Z_0, T)$	D H D	D H D	- - -
5	$[\Gamma_2(Y, T; Y_{i+1})-\Gamma_2(Y, T; Y_i)][\Gamma_2(Z, T; Z_{i+1})-\Gamma_2(Z, T; Z_i)]$	D H H	D H H	- - -
6	$[\Gamma_2(Y, T; Y_{i+1})-\Gamma_2(Y, T; Y_i)]\Gamma_3(Z, T; Z_0)$	D H E	D H E	- - -
7	$\Gamma_3(Y, T; Y_0)\Gamma_1(Z-Z_0, T)$	D E D	D E D	- - -
8	$\Gamma_3(Y, T; Y_0)[\Gamma_2(Z, T; Z_{i+1})-\Gamma_2(Z, T; Z_i)]$	D E H	D E H	- - -
9	$\Gamma_3(Y, T; Y_0)\Gamma_3(Z, T; Z_0)$	D E E	D E E	- - -
10	$\Gamma_1(Y-Y_0, T)\Gamma_1(Z-Z_0, T)$	H D D	H D D	- - -
11	$\Gamma_1(Y-Y_0, T)[\Gamma_2(Z, T; Z_{i+1})-\Gamma_2(Z, T; Z_i)]$	H D H	H D H	- - -
12	$\Gamma_1(Y-Y_0, T)\Gamma_3(Z, T; Z_0)$	H D E	H D E	- - -
13	$[\Gamma_2(Y, T; Y_{i+1})-\Gamma_2(Y, T; Y_i)]\Gamma_1(Z-Z_0, T)$	H H D	H H D	- - -
14	$[\Gamma_2(Y, T; Y_{i+1})-\Gamma_2(Y, T; Y_i)][\Gamma_2(Z, T; Z_{i+1})-\Gamma_2(Z, T; Z_i)]$	H H H	H H H	H H H
15	$[\Gamma_2(Y, T; Y_{i+1})-\Gamma_2(Y, T; Y_i)]\Gamma_3(Z, T; Z_0)$	H H E	H H E	H H E
16	$\Gamma_3(Y, T; Y_0)\Gamma_1(Z-Z_0, T)$	H E D	H E D	- - -
17	$\Gamma_3(Y, T; Y_0)[\Gamma_2(Z, T; Z_{i+1})-\Gamma_2(Z, T; Z_i)]$	H E H	H E H	H E H
18	$\Gamma_3(Y, T; Y_0)\Gamma_3(Z, T; Z_0)$	H E E	H E E	H E E
19	$\Gamma_1(Y-Y_0, T)\Gamma_1(Z-Z_0, T)$	E D D	E D D	- - -
20	$\Gamma_1(Y-Y_0, T)[\Gamma_2(Z, T; Z_{i+1})-\Gamma_2(Z, T; Z_i)]$	E D H	E D H	- - -
21	$\Gamma_1(Y-Y_0, T)\Gamma_3(Z, T; Z_0)$	E D E	E D E	- - -
22	$[\Gamma_2(Y, T; Y_{i+1})-\Gamma_2(Y, T; Y_i)]\Gamma_1(Z-Z_0, T)$	E H D	E H D	- - -
23	$[\Gamma_2(Y, T; Y_{i+1})-\Gamma_2(Y, T; Y_i)][\Gamma_2(Z, T; Z_{i+1})-\Gamma_2(Z, T; Z_i)]$	E H H	E H H	E H H
24	$[\Gamma_2(Y, T; Y_{i+1})-\Gamma_2(Y, T; Y_i)]\Gamma_3(Z, T; Z_0)$	E H E	E H E	E H E
25	$\Gamma_3(Y, T; Y_0)\Gamma_1(Z-Z_0, T)$	E E D	E E D	- - -
26	$\Gamma_3(Y, T; Y_0)[\Gamma_2(Z, T; Z_{i+1})-\Gamma_2(Z, T; Z_i)]$	E E H	E E H	E E H
27	$\Gamma_3(Y, T; Y_0)\Gamma_3(Z, T; Z_0)$	E E E	E E E	E E E
<i>Circular Geometry</i>				
28	$\Gamma_4(Y, Z, T; r_{i+1})-\Gamma_4(Y, Z, T; r_i)$	D H	D H	- -
29	$\Gamma_5(Y, Z, T)$	D E	D E	-
30	$\Gamma_4(Y, Z, T; r_{i+1})-\Gamma_4(Y, Z, T; r_i)$	H H	H H	H H
31	$\Gamma_5(Y, Z, T)$	H E	H E	H E
32	$\Gamma_4(Y, Z, T; r_{i+1})-\Gamma_4(Y, Z, T; r_i)$	E H	E H	E H
33	$\Gamma_5(Y, Z, T)$	E E	E E	E E
<i>Spherical Geometry</i>				
34	-	-	$f_X f_Y f_Z$	$\lambda_{kx} \lambda_{ky} \lambda_{kz}$
35	-	-	H	H
			E	E

† D, H and E denote a Dirac, Heaviside, and exponential distribution, respectively, for the longitudinal or transversal directions. Variables Y, Z and T are to be specified according to the conditions listed in Section 3.2.

‡ Number of problem

Several specific examples in Chapter 5 illustrate the selection of NP and MP. The user need not be concerned with the selection of the longitudinal and transversal auxiliary functions, G and Γ , as specified in Table 4. These are automatically selected according to the value selected for NP. However, the geometry of the initial, boundary, and production conditions should be carefully described following the format spelled out in Appendix B.

Consider again the initial value problems illustrated in Figs. 2 through 5. There is a step change in the initial concentration in the longitudinal and transversal directions. It should be noted that the notation used in Figs. 2 through 5 differs from the equations in the text. The initial conditions for N3DADE should be specified according to the latter. Because the current program can only solve the problem for multiple solute pulses along one coordinate, the solution for the IVP sketched in Figs. 2 through 4 needs to be determined by executing the problem twice. In both cases we need to specify one solute pulse for each coordinate. The solution for these three problems is given by (101) and (102). For the problems shown in Figs. 2 and 3 we need to select NP=14, whereas NP=30 for the cylindrical initial distribution in Fig. 4.

For Fig. 2 the problem needs to be solved twice, viz. for the upper and the lower slab; the conditions for each problem are:

$$f(X, Y, Z) = \begin{cases} f_1 & X_1 < X < X_2 \quad -\infty < Y < Y_2 \quad -\infty < Z < Z_2 \\ 0 & \text{otherwise} \end{cases} \quad (134)$$

where Y_1 and Z_1 are equal to zero for solving the problem associated with the upper slab. A solution for the problem shown in Fig. 3 is determined by adding the results, obtained for the upper and lower initial region that are each defined by:

$$f(X, Y, Z) = \begin{cases} f_1 & X_1 < X < X_2 \quad Y_1 < Y < Y_2 \quad Z_1 < Z < Z_2 \\ 0 & \text{otherwise} \end{cases} \quad (135)$$

Solution of the problem with two initial cylindrical regions depicted in Fig. 4, requires that we add results obtained for initial conditions of the form:

$$f(X, Y, Z) = \begin{cases} f_1 & X_1 < X < X_2 \quad 0 < r_c < r_1 \\ 0 & \text{otherwise} \end{cases} \quad (136)$$

The solution for the cylindrical problem is still given by (101) and (102), but the auxiliary transverse function is now defined by $\Gamma_4(Y, Z, T; r_i)$ (cf. Table 4).

Finally, for the problem shown in Fig. 5, we only need to execute the program once for two solute pulses since there is only one (spherical) coordinate. The expressions for the equilibrium and nonequilibrium solutions are given by (108) and (109) with associated auxiliary function $\Gamma_6(\xi, Y, Z, T; r_i)$. The numerical evaluation of this solution is very time consuming because of the multiple integration. The user needs to specify the center of the sphere, and two solute pulses according to:

$$f_X(X)f_Y(Y)f_Z(Z) = \begin{cases} f_1 & 0 < r_s < r_1 \\ f_2 & r_1 < r_s < r_2 \\ 0 & \text{otherwise} \end{cases} \quad (137)$$

4. PROGRAM DESCRIPTION

In this chapter we will review the general structure of the FORTRAN program N3DADE for evaluating the solutions that were presented in Chapter 3. The names of some of the main variables in the computer program are given in Appendix A (see also corresponding variables in the list of symbols). The preparation of the input file is documented in Appendix B. Careful attention should be paid to this issue because the program does not have a user-friendly pre-processor. Examples of input and output files are given in Appendices C and D, respectively. These files correspond to the examples discussed in Chapter 5. A broad outline of the different functions and routines in the program will be provided, while a complete listing of the code can be found in Appendix D.

4.1. Input Structure

The structure of the input file is documented in Appendix B. Five columns can be distinguished in Appendix B: (1) the line or row number in the input file, (2) the column numbers where data should be entered, (3) the format in which the variable is read in, (4) the variable name, and (5) comments. The user may, of course, change the input format by changing the source code to make preparation of the input file more convenient for his/her application (e.g., by using a free format or by limiting the number of options which are defined by parameters like MP, MC, NP).

The first five lines of the input file are common to all problems, but specification of the remaining lines will be different for a boundary, initial, or production value problem, depending also on the transversal conditions. The number of cases (NC) and the number of intervals in the Gauss-Chebyshev quadrature (NGC) for evaluating integrals are specified in the first line. The program can be executed for an arbitrary number of problems as specified by NC. The program processes the different cases sequentially. Line 1 is specified once while the information for lines 2 through 14 in Appendix B should be repeated NC times. Normally NC=1, but Appendix C shows one input file that allows the program to execute several problems. A minimum value for NGC of 50 should be sufficient to ensure accurate results for most transport problems. N3DADE is notoriously slow in handling the multiple integrations and the user may want to select a lower value for NGC to speed up the computations. The second line constitutes a comment on the problem; this comment will also

appear in the output file. The pore-water velocity, dispersion coefficient, and retardation factor are specified in line 3, the nonequilibrium parameters, β and ω , and the first-order decay coefficients are entered in line 4. We emphasize here that only the nonequilibrium parameters are dimensionless, the value of all other variables should conform to a consistent set of units. The program internally transforms the input variables to dimensionless parameters as specified in Table 1. The fifth line includes a reference length and the concentration used for transformation into dimensionless variables, the problem mode to distinguish between a boundary (BVP), initial (IVP), or production (PVP) value problem, and the concentration mode.

Lines 6 through 8 of the input file deal with the longitudinal transport problem. Line 6 is used as a header for either the BVP, IVP, or PVP. First, consider the input requirements for the BVP. The characteristics of the longitudinal and transversal conditions are determined by the problem number ($1 < NP < 33$), which is specified in line 7 in a manner consistent with Table 4 or the last part of Appendix B. The number of pulses for a Heaviside type of solute application needs to be provided in line 7 with respect to time, *and* with respect to the transversal directions y and z where applicable. The information entered in line 8 is different for a Dirac, Heaviside, and an exponential input; the program selects the input function according to the value for NP. For a Dirac type input the variable m denotes the mass of solute that is applied per unit cross sectional area of liquid filled pore space (i.e., the product of volumetric water content and area of porous medium) divided by the reference length, L . Note that the program needs to be modified to handle more than four input pulses for a Heaviside input. The program assumes that the first pulse is applied at $t=0$. Because the final time of a solute pulse is automatically the initial time of the following pulse, pulses of zero concentration have to be defined for the application of solute free water. No zero-concentration pulses exist for the transverse direction.

The IVP is considered next. The problem number and, if applicable, the number of solute pulses in the x , y , and z direction are entered in line 7. According to Table 4 or the last part of Appendix B, 35 different initial distributions can be selected including a Heaviside and an exponential distribution for a spherical geometry. For the data entry in line 8, a distinction is made between a Dirac (Eq.96), Heaviside (Eq.99), or exponential (Eq.103) distribution for either a rectangular or circular geometry, and a Heaviside (Eq.107) or exponential (Eq.110) distribution for a spherical

geometry. For instantaneous solute release in the x direction (Dirac function), the parameter m specifies the amount of solute mass initially present at $x=x_0$ per unit cross sectional area of water, divided by the reference length, L . The information for a Heaviside distribution depends on the number of pulses (including zero pulses) that are specified in line 7; unless the program is changed, only 80 characters can be read in (i.e., three pulses). If the initial concentration decreases exponentially with x , a maximum concentration, f_e [ML⁻³], and constant, α_e [L⁻¹], need to be specified. Problem numbers 34 and 35 concern a Heaviside and an exponential initial distribution with spherical symmetry about the point $(x_0, 0, 0)$. For a Heaviside distribution the (radial) distance from this point should be used for specifying the initial concentration. The number of initial pulses, NIP, should be equal to the number of shells plus one (i.e., the inner sphere). For an initial distribution that decreases exponentially away from the center $(x_0, 0, 0)$, the infinite limit for the spatial integrations in Eqs. (111) and (112) is approximated by the variable BINT.

The input for the evaluation of the PVP is similar to that of the IVP, except that no Dirac functions are included and that different production terms may be specified for the equilibrium and nonequilibrium phases. The problem number (NP=14,15,17,18,23,24,26,27,30-35) and, in case of the Heaviside problem the number of pulses, is specified in line 7. Data regarding the precise production profile are to be entered in line 8. Only two production pulses can be specified unless the input format of the program is changed.

The next data block pertains to specification of the transversal conditions as determined by the value of NP. In case of a rectangular geometry, information should be provided for the y -direction (line 9) and the z -direction (line 10). If the transversal conditions are described by a circular geometry, data should be entered in line 9 only. No data are needed for a spherical distribution because the IVP or PVP is completely described with the data entered in line 8. The number of transverse pulses for a Heaviside distribution is determined by the values for NYP (rectangular and circular geometry) and NZP (rectangular geometry only) in line 7. It is understood that a transverse pulse has a nonzero concentration or production.

The final block of data involves specification of the grid of independent variables for which the concentration needs to be calculated. This block starts at line 11 (rectangular geometry), line 10 (circular geometry), or line 9 (spherical geometry). The increment, the minimum, and the maximum

value for a particular variable (t , x , y , and z) should be specified in separate lines to define the proper solution domain. Four lines should also be used for a circular or spherical geometry since the dispersion coefficients may be different for the x , y , and z direction. Because the program requires more time to evaluate solutions for a circular and, especially, a spherical distribution, we recommend to limit the number of grid points for such cases. This can be done by accounting for possible symmetry of the problem and by not repeating the calculations once steady-state has been reached. Although the program is designed for three-dimensional problems, results can be conveniently obtained also for one- or two-dimensional problems. The increment for the "redundant" direction should then be set to zero or the same minimum and maximum value for that particular independent variable should be entered. Furthermore, a Heaviside condition with pulse boundaries sufficiently far from the minimum value of the variable should be specified.

4.2. Program Structure

As noted, examples of input and corresponding output files are listed in Appendices C and D, respectively. Appendix E contains a listing of the program N3DADE.FOR. The program contains a main section, the subroutine MODELS to calculate concentrations, a group of functions for solution of the one-dimensional BVP, IVP, and PVP as discussed in section 3.2, a group of functions to evaluate the longitudinal auxiliary expressions in Table 2, a group of functions to evaluate the transverse expressions in Table 3, routines for the Gauss-Chebyshev quadrature, and subroutines to calculate special functions.

In the main section a number of common blocks are declared; these blocks are used throughout the program. The names of the input and output files are defined through screen input (default names are N3DADE.IN and N3DADE.OUT). The input file, which was already discussed in section 4.1, is subsequently read in. Input variables are always transformed to dimensionless entities. The program is designed to solve one BVP, IVP, or PVP for a particular transversal distribution at the time. The user may modify N3DADE as needed to add results of individual problems according to the superposition principle to obtain concentrations for more complicated cases. Each time a point of the (t,x,y,z) grid is generated according to the input information, the program calls the subroutine models to calculate the equilibrium and nonequilibrium concentration for that point, and writes the

results to the output file.

In the subroutine MODELS, the equilibrium and nonequilibrium concentrations are calculated for the BVP (Dirac, Heaviside, or exponential functions), the IVP (Dirac, Heaviside, or exponential functions for a rectangular geometry and a Heaviside or exponential function for a spherical geometry), and the PVP (Heaviside or exponential functions for a rectangular geometry and a Heaviside or exponential function for a spherical geometry). The concentrations are calculated as the product of the one-dimensional nonequilibrium solution, and the transversal and longitudinal auxiliary functions. The subroutine calls the proper functions and integration routines, and sets boundaries for Heaviside distributions.

Following subroutine MODELS is a fairly long list of functions for more detailed evaluations and integration of specific expressions. The first group of functions pertains to equilibrium and nonequilibrium solutions for the one-dimensional BVP, IVP, and PVP. The acronyms for the function name indicate the type of: (1) function (DI=Dirac, H or HE=Heaviside, E or EX=exponential), (2) concentration (1=equilibrium, 2=nonequilibrium), (3) if applicable, geometry (S=spherical while an integration counter may be given), and (4) problem (B=BVP, I=IVP, P=PVP). The second group of functions evaluates the longitudinal auxiliary expressions. The acronyms for the functions follow the notation of Table 2. The third group of functions consists of transversal auxiliary functions given in Table 3. The transversal distribution may be described by a Dirac, Heaviside, or exponential function. The more complicated distributions involving a circular or spherical geometry, will require several steps leading to the transversal distribution. The integration routines use external functions, while evaluation of multiple integrals requires again a multistep approach. In the final group of functions, N3DADE evaluates the complementary error function, modified Bessel functions, Goldstein's J -function, and the two functions used for the exponentially decreasing input scenario.

5. EXAMPLES

Application of N3DADE will be illustrated in this chapter for five different examples. Graphical results are given for each example whereas the corresponding input and (abbreviated) output files are given in Appendices C and D, respectively. The selected examples are relatively generic and are not intended to cover all possible applications of the program. The choice of the parameter values and dimensions is also somewhat arbitrary. We will use dimensional parameters in most cases; any consistent set of units may be used (e.g., length in centimeters, time in days, mass in milligram).

5.1. Instantaneous Solute Application from a Disk

First, we consider the effect of the transfer rate parameter, ω , for instantaneous solute application from a disk at the surface of the soil or other porous medium. The flux-averaged concentration is predicted for three different mass transfer rates ($\omega=0.1, 1$, and 10) assuming the same partitioning coefficient $\beta=0.50$. This problem is modeled as a boundary value problem (MP=1) with a Dirac function for the input function, g_T , and a Heaviside function for the transverse input distribution, $g_Y g_Z$ for a circular geometry ($r_c=2.5$). According to Table 4 or Appendix B the problem number, NP, should be set to 28. The solution of the problem is based on (81) with $G(X, \tau)$ from Table 2b and $\Gamma_4(Y, Z, T, r)$ from Table 3. Calculations for this problem are relatively slow because of the many numerical integrations associated with the circular geometry. Solute adsorption is quantified with a retardation factor of 5. Additional parameters are $v=20$, $D_x=10$, $D_y=D_z=2.5$, $\mu_1=\mu_2=0$, $L=50$, and $c_0=1.0$. At $t=0$, a mass $m=20$ will be applied per unit cross-sectional area of soil water. For example, if the volumetric water content were 0.5, we would have to apply 196.35 mg of solute to a circular area at the surface of the medium with radius 2.5 cm. The corresponding input files, ONEA.IN and ONEB.IN, are listed in Appendix C. The problem is solved sequentially for three different ω .

Figure 6 shows C_1 as a function of time, t , at $x=50, y=z=0$ for $\omega=0.1, 1$, and 10 . Such curves have already been discussed for one-dimensional nonequilibrium transport [van Genuchten and Wierenga, 1976; Toride *et al.*, 1995]. The time for exchange between phases 1 and 2 is inversely proportional to ω . Breakthrough occurs at approximately $t=12.5$ (i.e., RL/v) if conditions are close to equilibrium (i.e., $\omega=10$). When ω is made smaller, some of the solute moves rapidly through the

soil without transfer to the nonequilibrium phase, resulting in early breakthrough with an increasingly higher peak concentration, whereas the remainder of the solute appears in the nonequilibrium phase and returns only slowly to the equilibrium phase, causing a long tail in the breakthrough curve.

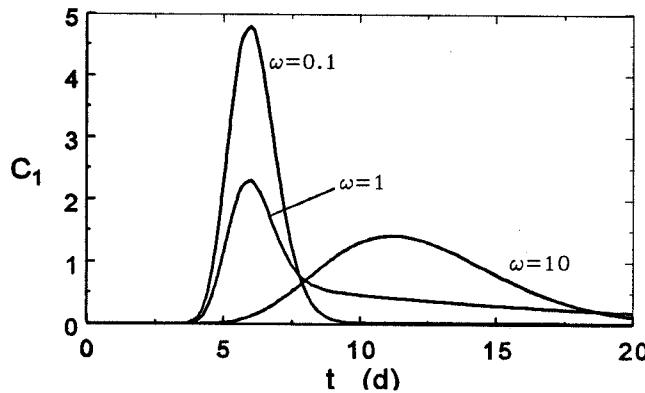


Fig. 6. Breakthrough curves for three different mass transfer coefficients resulting from instantaneous solute application.

We further investigated the concentration as a function of radial distance. Figure 7 shows C_1 in the transverse plane at $x=50$ for $t=6$ and 12. Figure 7a contains radial concentration profiles for the three transfer rates. The corresponding concentration contours are plotted in Fig. 7b. The contours are symmetric about $y=0$ and $z=0$. The solute moves initially at a fast pace for a low transfer rate, as demonstrated by the high values for $\omega=0.1$ at $t=6$. Conversely, the concentration is highest for $\omega=10$ at $t=12$. This behavior follows directly from the one-dimensional nonequilibrium transport behavior and was already illustrated in Fig. 6.

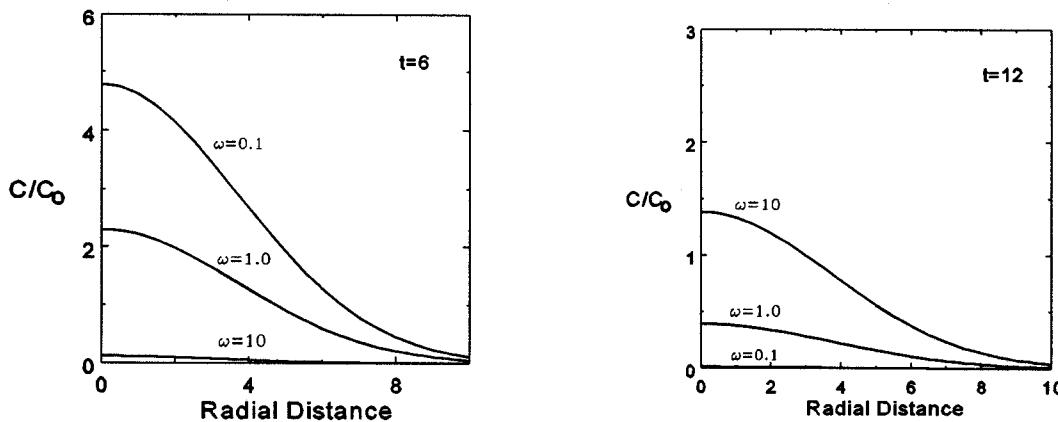


Fig. 7a. Transverse C_1 profiles at $x=50$ for three different mass transfer coefficients at $t=6$ and 12 resulting from instantaneous solute application to a circular area.

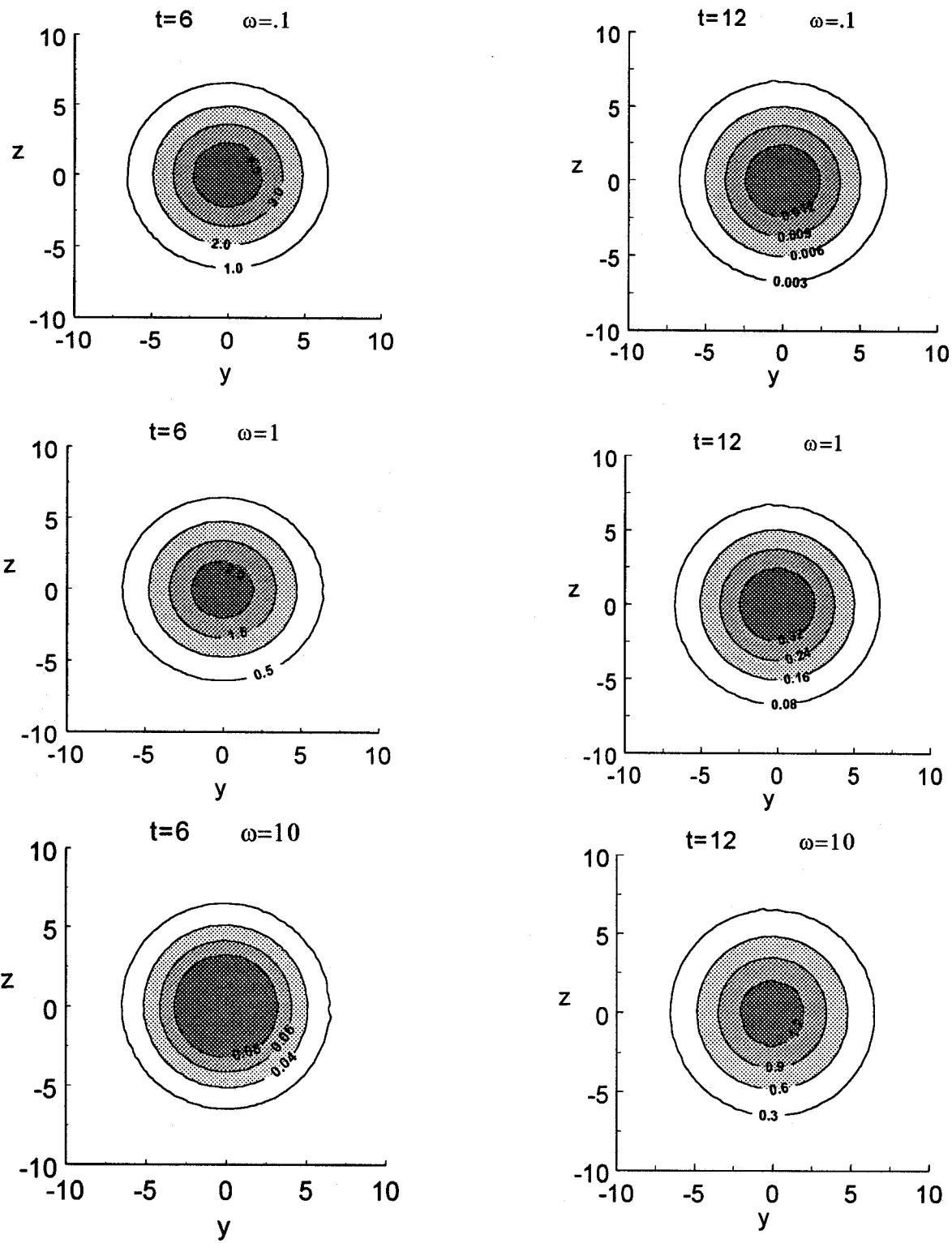


Fig. 7b. Contours for C_1 in the transversal plane at $x=50$ for three different mass transfer coefficients at $t=6$ and 12 resulting from instantaneous solute application to a circular area.

5.2. Continuous Solute Application from a Rectangle

The second example deals with the effect of an anisotropic transverse dispersion coefficient on the resident concentration for continuous solute application from a rectangular area at the surface. The input files TWOA.IN and TWOB.IN for this problem are again given in Appendix C. Dimensionless nonequilibrium parameters are $\omega=0.25$ and $\beta=0.50$. The problem is modeled as a boundary value problem ($MP=1$) with a Heaviside function for the input function, g_T , and a Heaviside function for the transverse input distribution, $g_Z g_Z$, using $NP=14$ (cf. Table 4). The solution for the two concentrations is given by (84) and (86), respectively, with $G(X, \tau)$ from Table 2a and $\Gamma_2(Y, T; Y)$ and $\Gamma_2(Z, T; Z)$ from Table 3. A step input is simulated by specifying a unit-pulse for $0 < t < 20$ (although any "large" upper limit could have been selected) to a rectangle at $x=0$ with $-2.5 < y < 2.5$ and $-2.5 < z < 2.5$. The dimensional "equilibrium" parameters are as follows: $R=4$, $v=20$, $D_x=20$, $D_y=10$, $D_z=5$, $\mu_1=\mu_2=0$, $L=20$, and $c_0=1.0$.

Figure 8 shows C_1 and C_2 versus longitudinal distance for times $t=5$, 10 , and 15 for $y=z=0$. Notice that the equilibrium concentration is almost identical for all three times, especially for small x . The nonequilibrium concentration increases with time until, at steady state, the equilibrium value will be reached. Notice also that the highest concentrations occur close to the inlet surface, but a decrease occurs with depth because of transverse dispersion.

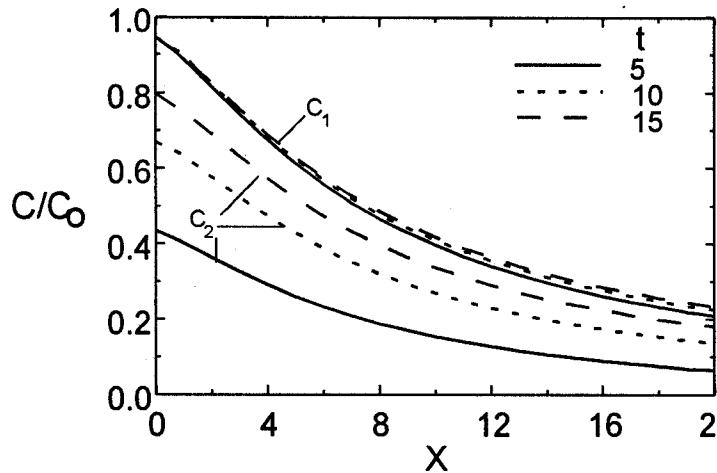


Fig. 8. C_1 and C_2 versus longitudinal distance at three different times resulting from continuous solute application to a rectangular surface area.

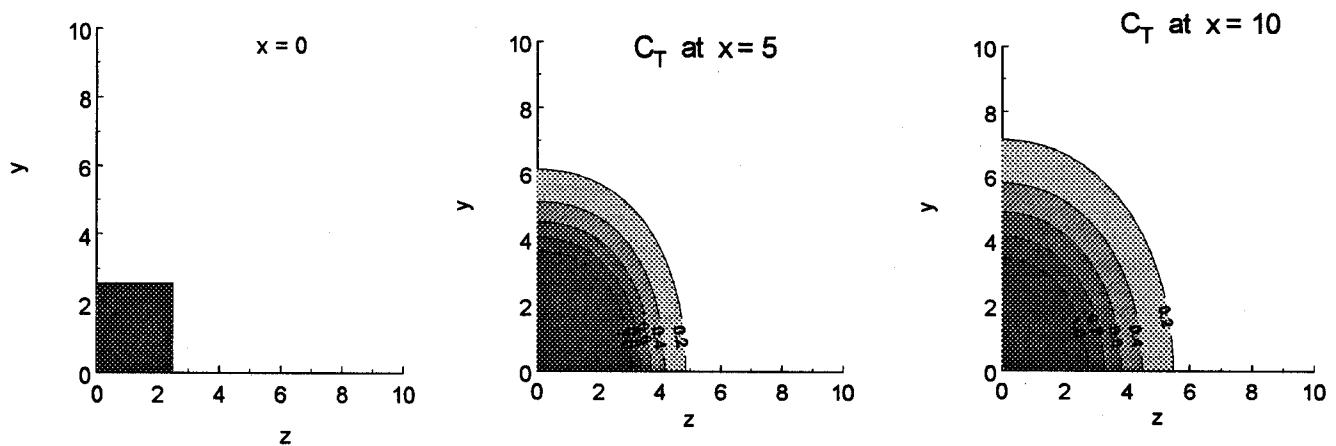


Fig. 9. Steady-state contours of the total concentration in the transverse plane at three longitudinal positions resulting from continuous solute application to a rectangular surface area.

Figure 9 shows contours in the yz plane of the total concentration at three longitudinal positions once steady state has been reached. The high-concentration area for $x=0$ directly corresponds to the inlet geometry. When the distance increases to $x=5$ and 10, the area with the maximum concentration decreases, while the solute is being spread over a larger cross-sectional area. Dispersion quickly smooths out sharp concentration gradients. Since the D_y -value is twice the D_z -value, the solute front extends farther in the y direction for all concentrations.

5.3. Rectangular Initial Value Problem

Consider the initial value problem ($MP=2$) sketched in the upper part of Figure 10 ($t=0$) where the solute is originally located in the regions $x_1=5 < x < x_2=15$ ($f_1=1$) and $x_3=25 < x < x_4=35$ ($f_3=0.5$) for $15 < y < 25$ and $-100 < z < 100$. The problem is two-dimensional for the domain of interest. The initial profile is given by Heaviside functions in the longitudinal and transversal directions ($NP=14$). The equilibrium and nonequilibrium concentrations are now given by (101) and (102), respectively, with $G(X, T; X_i)$ from Table 2a and $\Gamma_2(Y, T; Y_j)$ and $\Gamma_2(Z, T; Z_j)$ from Table 3. The input file THREE.IN is given in Appendix C. Equilibrium parameters are: $v=50$, $R=1$, $D_x=20$, $D_y=D_z=5$, $\mu_1=\mu_2=0$, $L=100$, and $c_0=1.0$. The nonequilibrium parameters are $\beta=0.5$ and $\omega=1$. The remainder of Fig. 10 consists of plots for C_1 , C_2 , and C_T at $t=0.5$.

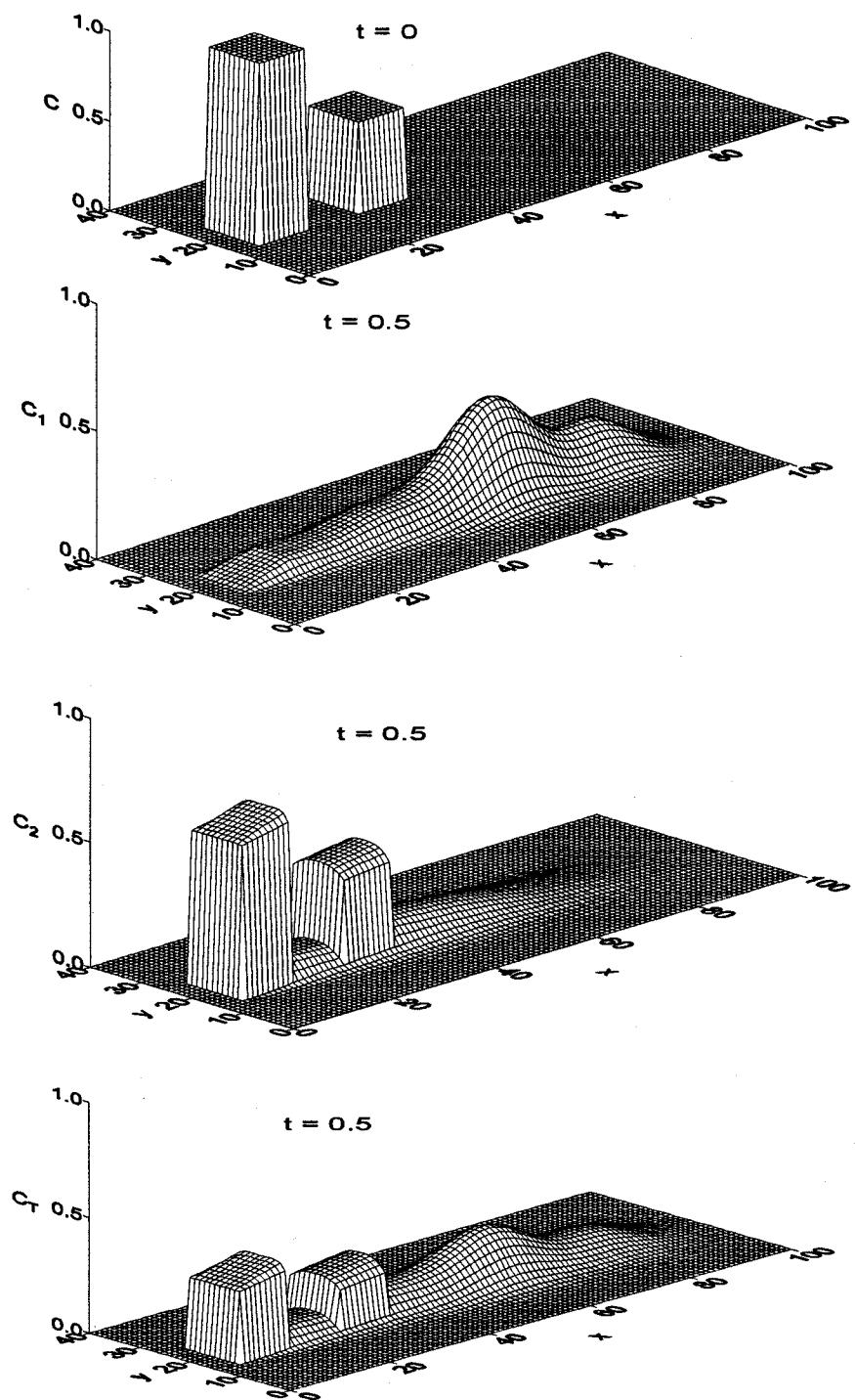


Fig. 10. Initial concentration and C_1 , C_2 , and C_T at $t=0.5$ as a function of longitudinal and transversal (y) direction for a nonreactive solute with $\beta=0.5$ and $\omega=1$.

The equilibrium concentration, C_1 , follows a predictable pattern: the solute moves downstream as a result of advection, but with the initially distinct peaks being blurred due to dispersion. Because of nonequilibrium exchange, solute remains in the mobile region across a large part of the x -direction. The C_2 profile is still quite similar to the initial distribution; the solute can move only through transport in the mobile region and subsequent transfer into the immobile region. Finally, the total concentration, C_T consists of weighted contributions from the equilibrium and nonequilibrium concentrations. It is apparent that the complete displacement of solutes from the soil profile is difficult to achieve as a result of nonequilibrium phenomena.

5.4. Spherical Initial Value Problem

The fourth example also pertains to an initial value problem. We assume that the solute has initially a maximum value at the point given by $x=x_0=5$, $y=0$, and $z=0$. The solute concentration decreases exponentially according to (110) with $\alpha=2$ and $f_e=1$. The resident concentrations for the equilibrium and nonequilibrium phases are given by (111) and (112). The corresponding input file FOUR.IN is shown in Appendix C. Equilibrium transport parameters are as follows: $v=5$, $R=1$, $D_x=10$, $D_y=D_z=5$, $\mu_1=\mu_2=0$, $L=20$, and $c_o=1.0$. The nonequilibrium parameters are again $\beta=0.5$ and $\omega=1$. The solution of this problem requires many computations. To limit computer time we reduced the number of points in the Gauss-Chebyshev quadrature (NGC) to 20. Figure 11 shows the contours for C_1 , C_2 , and C_T at $t=1$ in the xy -plane. Because of symmetry any radial distance from the x -coordinate may be selected for y . The equilibrium concentration, C_1 , moves relatively fast through the medium ahead of the center of mass predicted with equilibrium theory ($vt/R+x_0=10$). Solute is spread out over a larger area downstream than upstream from the initial center of mass. The nonequilibrium concentration shows less movement; the profile still resembles the initial distribution.

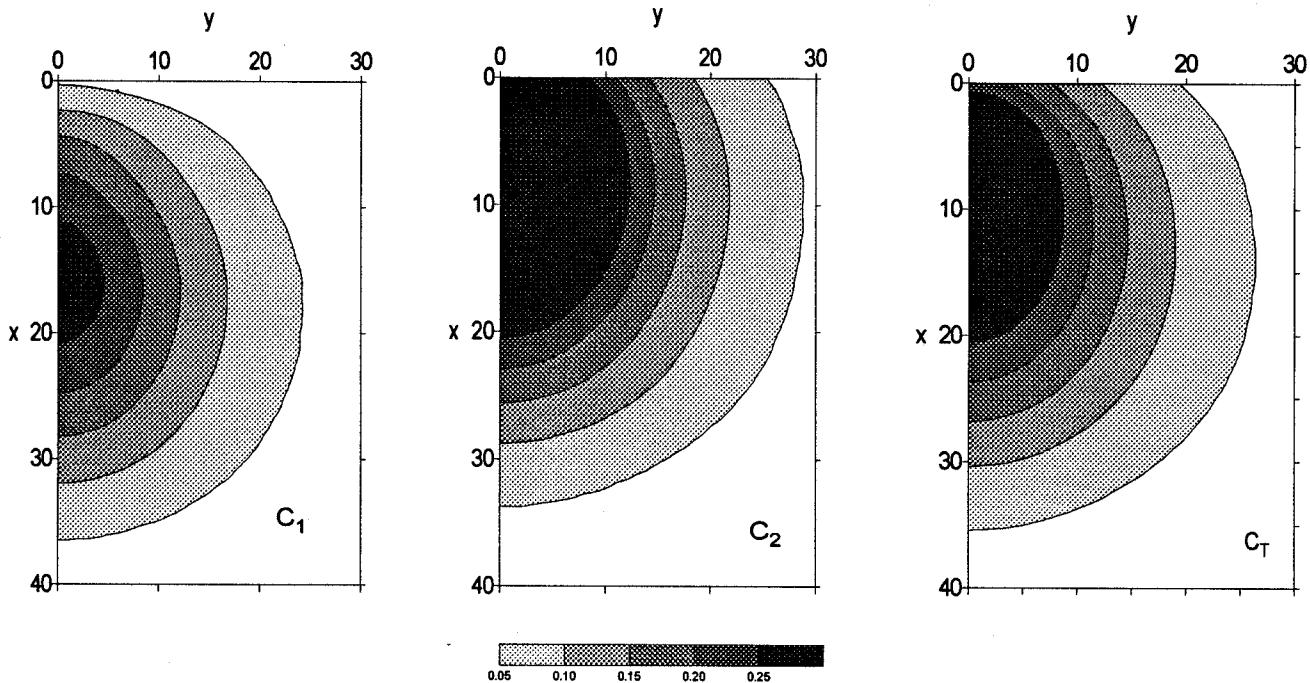


Fig. 11. Contours of C_1 , C_2 , and C_T in the xy -plane at $z=0$ and $t=1$ for an initial concentration that decreases exponentially in a hypothetical sphere with center $x=5$, $y=0$, and $z=0$.

5.5. Cylindrical Production Value Problem

The final example involves solute production in a cylindrical region of the soil ($0 < x < 10$ and $0 < r_c$ or $y < 2.5$). The problem is modeled as a production value problem (MP=3) with a Heaviside function for the longitudinal and transversal directions (NP=30). The analytical solutions for the equilibrium and nonequilibrium concentrations are given by Eqs.(114) and (115), respectively, while the total concentration is defined by (12). The longitudinal auxiliary function, $G(X, \tau, X_i)$, is given in Table 2a and $\Gamma_2(Y, Z, T, r_i)$ is defined in Table 3. The input file FIVE.IN in Appendix C specifies all the input variables. The production factors are $\lambda_1=0.5$ and $\lambda_2=1$. Equilibrium parameters are $v=5$, $R=1$, $D_x=5$, $D_y=D_z=2$, $\mu_1=0.5$, $\mu_2=0$, $L=20$, and $c_o=0.25$ with nonequilibrium parameters $\beta=0.5$ and $\omega=5$. The value for NGC is set to 20. Figure 12 shows the contours for C_1 , C_2 , and C_T at steady state (e.g. $t=20$) in the xy -plane. The equilibrium concentration, C_1 , increases along the axis of the hypothetical cylinder from $x=0$ to about $x=8$; solute that is produced upstream moves down and adds to the solute that is produced downstream. The concentration decreases beyond $x=8$ because of transverse

dispersion and, more importantly, first-order solute decay in the equilibrium phase. The maximum value for the nonequilibrium concentration occurs roughly in the cylindrical region where solute production occurs. Because λ_2 is twice as large as λ_1 , C_2 tends to be higher than C_1 while the solute in the nonequilibrium phase extends to a relatively large area due to the high transfer rate between the equilibrium and nonequilibrium phases. The total concentration follows directly from the equilibrium and nonequilibrium concentrations. It should be noted that if solute is applied to the soil surface, or if solute is already present at $t=0$, we also need to independently solve a BVP or IVP; summation of the results yields the concentration according to the superposition principle. Because λ_2 is twice as large as λ_1 , C_2 tends to be higher than C_1 while the solute in the nonequilibrium phase extends to a relatively large area due to the high transfer rate between the equilibrium and nonequilibrium phases. The total concentration follows directly from the equilibrium and nonequilibrium concentrations. It should be noted that if solute is applied to the soil surface, or if solute is already present at $t=0$, we also need to independently solve a BVP or IVP; summation of the results yields the concentration according to the superposition principle.

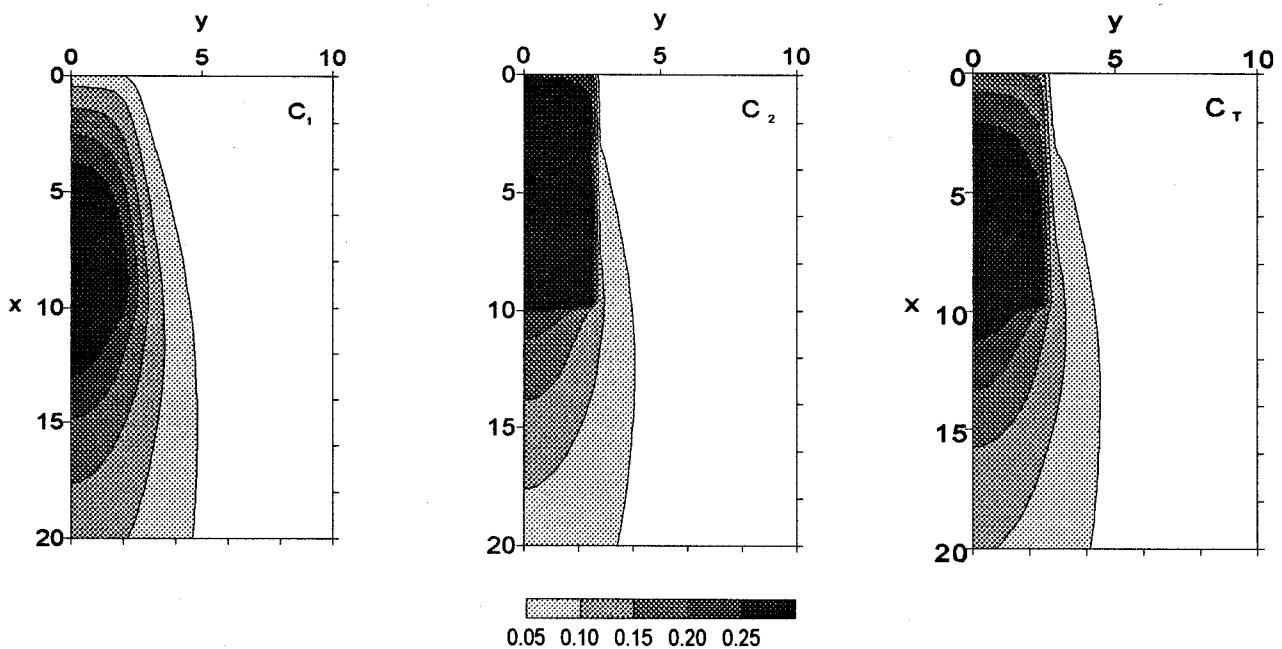


Fig. 12. Steady-state contours of C_1 , C_2 , and C_T in the xy -plane at $z=0$ for solute production in a hypothetical cylinder with $0 < x < 10$ and $0 < r < 2.5$.

6. REFERENCES

- Brusseau, M. L., R. E. Jessup, and P. S. C. Rao. 1989. Modeling the transport of solutes influenced by multi-process nonequilibrium. *Water Resour. Res.* 25:1971-1988.
- Cameron, D. A., and A. Klute. 1977. Convective-dispersive solute transport with a combined equilibrium and kinetic adsorption model. *Water Resour. Res.* 19:718-724.
- Coats, K. H., and B. D. Smith. 1964. Dead-end pore volume and dispersion in porous media. *Soc. Petrol. Eng. J.* 4:73-84.
- De Smedt, F., and P. J. Wierenga. 1979a. A generalized solution for solute flow in soils with mobile and immobile water. *Water Resour. Res.* 15:1137-1141.
- De Smedt, F., and P. J. Wierenga. 1979b. Mass transfer in porous media with immobile water. *J. Hydrol.* 41:59-67.
- Goldstein, S. 1953. On the mathematics of exchange processes in fixed columns. I. Mathematical solutions and asymptotic expansions. *Proc. Roy. Soc. London A* 219:151-185.
- Goltz, M. N., and P. V. Roberts. 1986. Three-dimensional solutions for solute transport in an infinite medium with mobile and immobile zones. *Water Resour. Res.* 22:1139-1148.
- Gradshteyn, I. S., and I. M. Ryzhik. 1980. *Table of integrals, series, and products*. Academic Press, San Diego, 1160 pp.
- Hiester, N. K., and T. Vermeulen. 1952. Saturation performance of ion-exchange columns and adsorption columns. *Chem. Eng. Prog.* 48:505-516.
- Klinkenberg, A. 1948. Numerical evaluation of equations describing transient heat and mass transfer in packed solids. *Ind. Eng. Chem.* 40:1992-1994.
- Kreft, A., and Zuber, A. 1978. On the physical meaning of the dispersion equation and its solutions for different initial and boundary conditions. *Chem. Eng. Sci.* 33:1471-1480.
- Lassey, K. R. 1982. On the computation of certain integrals containing the modified Bessel function $I_0(\xi)$. *Math. Comp.* 39:625-637.
- Lassey, K. R. 1988. Unidimensional solute transport incorporating equilibrium and rate-limited isotherms with first-order loss. 1. Model conceptualizations and analytic solutions. *Water Resour. Res.* 3:343-350.
- Leij, F.J., and S.A. Bradford. 1994. 3DADE: A computer program for evaluating three-dimensional equilibrium solute transport in porous media. Research Report 134, U.S. Salinity Laboratory, Riverside, CA.
- Leij, F. J., T. H. Skaggs, and M. Th. van Genuchten. 1991. An analytical solutions for solute transport in three-dimensional semi-infinite porous media. *Water Resour. Res.* 27:2719-2733.
- Leij, F. J., N. Toride, and M. Th. van Genuchten. 1993. Analytical solutions for non-equilibrium solute transport in three-dimensional porous media. *J. Hydrol.* 151:193-228.
- Lindstrom, F. T., and W. M. Stone. 1974. On the start up or initial phase of linear mass transport of chemicals in a water saturated sorbing porous medium: 1., *SIAM J. Appl. Math.*, 26, 578-591.
- Luke, Y. L. 1962. *Integrals of Bessel functions*. McGraw-Hill, New York.

- Nkedi-Kizza, P., J. W. Biggar, M. Th. van Genuchten, P. J. Wierenga, H. M. Selim, J. M. Davidson, and D. R. Nielsen. 1983. Modeling tritium and chloride 36 transport through an aggregated Oxisol. *Water Resour. Res.* 19:691-700.
- Nkedi-Kizza, P., J. W. Biggar, H. M. Selim, M. Th. van Genuchten, P. J. Wierenga, J. M. Davidson, and D. R. Nielsen. 1984. On the equivalence of two conceptual models for describing ion exchange during transport through an aggregated oxisol. *Water Resour. Res.* 20:1123-1130.
- Olver, F.W.J. 1965. Bessel functions of integer order. In M. Abramowitz and I.A. Stegun (Editors) *Handbook of Mathematical Functions*. pp. 355-433. Dover Publishing Co., New York.
- Parker, J.C., and M. Th. van Genuchten. 1984. Flux-averaged and volume-averaged concentrations in continuum approaches to solute transport. *Water Resour. Res.* 20:866-872.
- Selim, H. M., J. M. Davidson, and R. S. Mansell. 1976. Evaluation of a two-site adsorption-desorption model for describing solute transport in soils. In Proc. Summer Computer Simulation Conf., Washington, D.C.
- Spiegel, M. R. 1965. *Theory and problems of Laplace transforms*. Schaum's Outline Ser., McGraw-Hill, New York.
- Toride, N., F. J. Leij, and M. Th. van Genuchten. 1993. A comprehensive set of analytical solutions for nonequilibrium solute transport with first-order decay and zero-order production. *Water Resour. Res.* 29:2167-2182.
- Toride, N., F. J. Leij, and M. Th. van Genuchten. 1995. The CXTFIT code for estimating transport parameters from laboratory or field tracer experiments. Research Report 137, U.S. Salinity Laboratory, Riverside, CA.
- van Genuchten, M. Th., and J. C. Parker. 1984. Boundary conditions for displacement experiments through short laboratory soil columns. *Soil Sci. Soc. Am. J.* 48:703-708.
- van Genuchten, M. Th., and R. J. Wagenet. 1989. Two-site/two-region models for pesticide transport and degradation: theoretical development and analytical solutions. *Soil Sci. Soc. Am. J.* 53:1303-1310.
- van Genuchten, M. Th., and P. J. Wierenga. 1976. Mass transfer studies in sorbing porous media. I. Analytical solutions. *Soil Sci. Soc. Am. J.* 40:473-481.
- van Genuchten, M. Th., and P.J. Wierenga. 1977. Mass transfer studies in sorbing porous media. II. Experimental evaluation with tritium ($^3\text{H}_2\text{O}$). *Soil Sci. Soc. Am. Proc.* 41:272-278.
- Villermaux, J., and W. P. M. van Swaaij. 1969. Modèle représentatif de la distribution des temps de séjour dans un réacteur semi-infini à dispersion axiale avec zones stagnantes. Application à l'écoulement ruisselant dans des colonnes d'anneaux Raschig. *Chem. Eng. Sci.* 24:1097-1111.

APPENDIX A. MAIN PROGRAM VARIABLES

<i>Variable</i>	<i>Description</i>
ALB	Parameter in exponential input profile
ALI	Parameter in exponential initial distribution
ALP	Parameter in exponential production distribution
ALY	Parameter in transversal exponential distribution
ALZ	Parameter in transversal exponential distribution
BETA	Partition coefficient, β
BINT	Boundary value to approximate infinite limits of integration
CO	Arbitrary reference concentration, C_o
DCX	Longitudinal dispersion coefficient, D_x
DX(I)	Increments in x, y, z , and t , respectively, to specify nodes for which the concentration needs to be calculated.
DCY	Transversal dispersion coefficient, D_y
DCZ	Transversal dispersion coefficient, D_z
DMB	Mass for Dirac input profile
DMI	Mass for Dirac initial profile
FE	Factor in exponential decreasing initial profile
FP	Initial concentration for Heaviside profile, f_i
GE	Factor in exponentially decreasing input concentration, g_e
GP	Input concentration for Heaviside profile, g_i
MP	Mode of problem
MC	Mode of concentration
NC	Number of cases considered.
NGC	Number of intervals, n , in Gauss-Chebyshev quadrature
NBP	Number of pulses in Heaviside boundary profile
NIP	Number of pulses in Heaviside initial profile
NPP	Number of pulses in Heaviside production profile
NYP	Number of pulses in transverse direction
NZP	Number of pulses in transverse direction
OLAM	Factor in Heaviside production profile for equilibrium phase, λ_{1e}
OLAME	Factor in exponential production profile for equilibrium phase, λ_{1e}
OM1	$\omega/(1-\beta)R$
OM2	$\omega/\beta R$
OMEGA	Mass transfer coefficient, ω
OMOM	$\omega^2/[\beta(1-\beta)R^2]$
OMU1	$(\omega+\mu_1)/\beta R$
OMU2	$(\omega+\mu_2)/(1-\beta)R$
PX	Longitudinal Peclet number, P_x
PY	Transversal Peclet number, P_y
PZ	Transversal Peclet number, P_z

<i>Variable</i>	<i>Description</i>
R	Retardation factor
TITLE	Character string to identify problem.
TLAM	Factor in Heaviside production profile for nonequilibrium phase, λ_{2i}
TLAME	Factor in exponential production profile for equilibrium phase, λ_{2e}
T0	Application time for Dirac input, T_0
TP	Initial or final time of solute pulse for BVP
U1	μ_1
U2	μ_2
U1R	$\mu_1/\beta R$
U2R	$\omega\mu_2/[(\omega+\mu_2)\beta R]$
UL	Arbitrary reference length, L
V	Pore-water velocity
X	Dimensionless independent variable (T , X , Y , or Z)
XD	Dimensional independent variable (t , x , y , or z)
XLOW	Lower limit for t , x , y , and z for which concentration is to be calculated
X0	Initial position for Dirac distribution, X_0
XP	Initial or final position of solute pulse for IVP
XUP	Upper limit for t , x , y , and z for which concentration is to be calculated
Y1	Equilibrium concentration
Y2	Nonequilibrium concentration
YT	Total concentration
YD1	Dimensional equilibrium concentration
YD2	Dimensional nonequilibrium concentration
YDT	Dimensional total concentration
Y0	Position for transversal Dirac distribution, Y_0
Z0	Position for transversal Dirac distribution, Z_0

APPENDIX B. INPUT FILE STRUCTURE

<i>Line</i>	<i>Columns</i>	<i>Format</i>	<i>Variable</i>	<i>Comments</i>
1	1-5	I5	NC	The number of cases considered. The remaining lines are read in for each case.
	6-10	I5	NGC	Number of intervals for Gauss-Chebyshev quadrature
2	1-60	A60	TITLE	Comment to describe problem and list dimensions
3	1-10	F10.2	V	Value for $v (>0)$
	11-20	F10.2	R	Value for $R (>0)$
	21-30	F10.2	DCX	Value for $D_x (>0)$
	31-40	F10.2	DCY	Value for $D_y (>0)$
	41-50	F10.2	DCZ	Value for $D_z (>0)$
4	1-10	F10.2	BETA	Value for $\beta (0 < \beta < 1)$
	11-20	F10.2	OMEGA	Value for $\omega (>0)$
	21-30	F10.2	U1	Value for μ_1
	31-40	F10.2	U2	Value for μ_2
5	1-10	F10.2	UL	Value for $L (>0)$
	11-20	F10.2	CO	Value for $C_o (>0)$
	21-30	I10	MP	Mode of problem (BVP:MP=1; IVP:=2; PVP:=3)
	31-40	I10	MC	Mode of concentration (flux-averaged:MC=1, volume-averaged:#1)

Boundary Value Problem (MP=1)

6	1-60	A60	TITLE	Identifying line for BVP
7	1-5	I5	NP	Code for number of problem (cf. Table 4)
	6-10	I5	NBP	Number of pulses with respect to t (only for Heaviside)
	11-15	I5	NYP	Number of pulses with respect to y (only for Heaviside)
	16-20	I5	NZP	Number of pulses with respect to z (only for Heaviside)

Dirac (NP=1-9,28,29)

8	1-10	F10.2	T0	Time of application, t_0
	11-20	F10.2	DMB	Applied mass in Dirac pulse, m

Heaviside (10-18,30,31)

8	F10.2	1-10	GP(1)	Concentration, g_1 , of first pulse ($0 < t < t_2$)
	F10.2	11-20	TP(2)	Final time of first pulse, t_2 (possibly initial time of second pulse)
	F10.2	21-30	GP(2)	Concentration, g_2 , of second pulse ($t_2 < t < t_3$)
	F10.2	31-40	TP(3)	Final time of second pulse, t_3 (possibly initial time of third pulse)
(Number of entries should be 2NBP)				

Exponential (19-27,32,33)

8	F10.2	1-10	GE	Concentration of exponential term, $g_e (t > 0)$
	F10.2	11-20	ALB	Parameter in exponential function, α

<i>Line</i>	<i>Columns</i>	<i>Format</i>	<i>Variable</i>	<i>Comments</i>
Initial Value Problem (MP=2)				
6	1-60	I60	TITLE	Identifying line for IVP
7	1-5	I5	NP	Code for type of problem (cf. Table 4)
	6-10	I5	NIP	Number of pulses with respect to x (only for Heaviside)
	11-15	I5	NYP	Number of pulses with respect to y (only for Heaviside)
	16-20	I5	NZP	Number of pulses with respect to z (only for Heaviside)
Dirac (NP=1-9,28,29)				
8	1-10	F10.2	X0	Location of application, x_0
	11-20	F10.2	DMI	Initial amount of mass in Dirac pulse, m
Heaviside (10-18,30,31)				
8	F10.2	1-10	XP(1)	Initial position of first pulse, x_1
	F10.2	11-21	FP(1)	Concentration, f_1 , of first pulse ($x_1 < x < x_2$)
	F10.2	21-30	XP(2)	Final position of first pulse, x_2 (possibly initial position of second pulse)
	F10.2	31-40	FP(2)	Concentration, f_2 , of second pulse ($x_2 < x < x_3$)
	F10.2	41-50	XP(3)	Final position of second pulse, x_3 (possibly initial position of third pulse)
(Number of entries should be 2NIP+1)				
Exponential (19-27,32,33)				
8	F10.2	1-10	FE	Concentration, f_e ($x > 0$)
	F10.2	11-20	ALI	Parameter in exponential function, α
<i>Spherical Geometry</i>				
Heaviside (34)				
8	F10.2	1-10	X0	Center of sphere, x_0
	F10.2	11-20	FP(1)	Concentration, f_1 , of first pulse ($0 < r < r_1$)
	F10.2	21-30	XP(1)	Radius of inner sphere, r_1
	F10.2	31-40	FP(2)	Concentration, f_2 , of second pulse ($r_1 < r < r_2$)
	F10.2	41-50	XP(2)	Outer radius of first shell, r_2
(Number of entries should be 2NIP+1)				
Exponential (35)				
8	F10.2	1-10	X0	Center of sphere, x_0
	F10.2	11-20	FE	Concentration, f_e ($x > 0$)
	F10.2	21-30	ALI	Parameter in exponential function, α
	F10.2	31-40	BINT	Boundary of integration

<i>Line</i>	<i>Columns</i>	<i>Format</i>	<i>Variable</i>	<i>Comments</i>
Production Value Problem (MP=3)				
6	1-60	I60	TITLE	Identifying line for PVP
7	1-5	I5	NP	Code for type of problem (cf. Table 4)
	6-10	I5	NPP	Number of pulses with respect to x (only for Heaviside)
	11-15	I5	NYP	Number of pulses with respect to y (only for Heaviside)
	16-20	I5	NZP	Number of pulses with respect to z (only for Heaviside)
Heaviside (NP=14,15,17,18,30,31)				
8	F10.2	1-10	XP(1)	Initial position of first pulse, x_1
	F10.2	11-20	OLAM(1)	Equilibrium production, λ_{1e} , of first pulse ($x_1 < x < x_2$)
	F10.2	21-30	TLAM(1)	Nonequilibrium production, λ_{21} , of first pulse
	F10.2	31-40	XP(2)	Final position of first pulse, x_2 (possibly initial position of second pulse)
	F10.2	41-50	OLAM(2)	Equilibrium production, λ_{12} , of second pulse ($x_2 < x < x_3$)
	F10.2	51-60	TLAM(2)	Nonequilibrium production, λ_{22} , of second pulse
	F10.2	61-70	XP(3)	Final position of second pulse, x_3 (possibly initial position of third pulse)
(Number of entries should be 3NPP+1)				
Exponential (23,24,26,27,32,33)				
8	F10.2	1-10	OLAME	Equilibrium production, λ_{1e} , of first pulse ($x_1 < x < x_2$)
	F10.2	11-20	TLAME	Nonequilibrium production, λ_{2e} , of first pulse
	F10.2	21-30	ALP	Parameter in exponential function, α
	F10.2	31-40	BINT	Boundary of integration
Spherical Geometry				
Heaviside (34)				
8	F10.2	1-10	X0	Center of sphere, x_0
	F10.2	11-20	OLAM(1)	Equilibrium production, λ_{11} , of first pulse ($0 < r < r_1$)
	F10.2	21-30	TLAM(1)	Nonequilibrium production, λ_{21} , of first pulse
	F10.2	31-40	XP(1)	Radius of inner sphere, r_1
	F10.2	41-50	OLAM(2)	Equilibrium production, λ_{12} , of second pulse ($r_1 < r < r_2$)
	F10.2	51-60	TLAM(2)	Nonequilibrium production, λ_{22} , of second pulse
	F10.2	61-70	XP(2)	Outer radius of first shell, r_2
(Number of entries should be 3NPP+1)				
Exponential (35)				
8	F10.2	1-10	X0	Center of sphere, x_0
	F10.2	11-20	OLAME	Equilibrium production, λ_{1e} ($x > 0$)
	F10.2	21-30	TLAME	Equilibrium production, λ_{2e} ($x > 0$)
	F10.2	31-40	ALP	Parameter in exponential function, α
	F10.2	41-50	BINT	Boundary of integration

<i>Line</i>	<i>Columns</i>	<i>Format</i>	<i>Variable</i>	<i>Comments</i>
Transversal Conditions (Omit for spherical geometry)				
Dirac-Dirac (1,10,19)				
9	1-10	F10.2	Y0	Position of application, y_0
10	1-10	F10.2	Z0	Position of application, z_0
Dirac-Heaviside (2,11,20)				
9	1-10	F10.2	Y0	Position of application, y_0
10	1-10	F10.2	ZP(1)	Position of start of first pulse, z_1
11-20	F10.2	ZP(2)		Position of end of first pulse, z_2
(Number of entries should be 2NZP)				
Dirac-Exponential (3,12,21)				
9	1-10	F10.2	Y0	Position of application, y_0
10	1-10	F10.2	ALZ	Parameter in exponential function, α
11-20	F10.2	Z0		Position of application, z_0
Heaviside-Dirac (4,13,22)				
9	1-10	F10.2	YP(1)	Position of start of first pulse, y_1
11-20	F10.2	YP(2)		Position of end of first pulse, y_2
(Number of entries should be 2NYP)				
10	1-10	F10.2	Z0	Position of application, z_0
Heaviside-Heaviside (5,14,23)				
9	1-10	F10.2	YP(1)	Position of start of first pulse, y_1
11-20	F10.2	YP(2)		Position of end of first pulse, y_2
(Number of entries should be 2NYP)				
10	1-10	F10.2	ZP(1)	Position of start of first pulse, z_1
11-20	F10.2	ZP(2)		Position of end of first pulse, z_2
(Number of entries should be 2NZP)				
Heaviside-Exponential (6,15,24)				
9	1-10	F10.2	YP(1)	Position of start of first pulse, y_1
11-20	F10.2	YP(2)		Position of end of first pulse, y_2
(Number of entries should be 2NYP)				
10	1-10	F10.2	ALZ	Parameter in exponential function, α
11-20	F10.2	Z0		Position of application, z_0

<i>Line</i>	<i>Columns</i>	<i>Format</i>	<i>Variable</i>	<i>Comments</i>
<u>Exponential-Dirac (7,16,25)</u>				
9	1-10	F10.2	ALY	Parameter in exponential function, α
	11-20	F10.2	Y0	Position of application, y_0
10	1-10	F10.2	Z0	Position of application, z_0
<u>Exponential-Heaviside (8,17,26)</u>				
9	1-10	F10.2	ALY	Parameter in exponential function, α
	11-20	F10.2	Y0	Position of application, y_0
10	1-10	F10.2	ZP(1)	Position of start of first pulse, z_1
	11-20	F10.2	ZP(2)	Position of end of first pulse, z_2 (Number of entries should be 2NZP)
<u>Exponential-Exponential (9,18,27)</u>				
9	1-10	F10.2	ALY	Parameter in exponential function, α
	11-20	F10.2	Y0	Position of application, y_0
10	1-10	F10.2	ALZ	Parameter in exponential function, α
	11-20	F10.2	Z0	Position of application, z_0
<i>Circular Geometry</i>				
<u>Heaviside (28,30,32)</u>				
9	F10.2	1-10	YP(1)	Starting radius of application area for first pulse, r_1
	F10.2	11-20	YP(2)	Ending radius of application area for first pulse, r_2 (Number of entries should be 2NYP)
<u>Exponential (29,31,33)</u>				
9	F10.2	1-10	ALY	Parameter in exponential function, α
	F10.2	11-20	BINT	Boundary of integration
<u>Node Spacing†</u>				
11	F10.2	1-10	DX(1)	Increment in t
	F10.2	11-20	XLOW(1)	Lower limit of t
	F10.2	21-30	XUP(1)	Upper limit of t
12	F10.2	1-10	DX(2)	Increment in x
	F10.2	11-20	XLOW(2)	Lower limit of x
	F10.2	21-30	XUP(2)	Upper limit of x
13	F10.2	1-10	DX(3)	Increment in y
	F10.2	11-20	XLOW(3)	Lower limit of y
	F10.2	21-30	XUP(3)	Upper limit of y
14	F10.2	1-10	DX(4)	Increment in z
	F10.2	11-20	XLOW(4)	Lower limit of z
	F10.2	21-30	XUP(4)	Upper limit of z

† Decrease line number by 1 for cylindrical and by 2 for spherical geometry

Listing of Numbers and Modes of Problems

NP	MP	Description
<i>Rectangular Geometry</i>		
1	1,2	Dirac function for x, y and z directions
2	1,2	Dirac function for x and y directions, Heaviside function for z direction
3	1,2	Dirac function for x and y directions, exponential function for z direction
4	1,2	Dirac function for x and z directions, Heaviside function for y direction
5	1,2	Dirac function for x direction, Heaviside function for y and z directions
6	1,2	Dirac function for x , Heaviside function for y , exponential function for z direction
7	1,2	Dirac function for x and z directions, exponential function for y direction
8	1,2	Dirac function for x , exponential function for y , Heaviside function for z direction
9	1,2	Dirac function for x direction, exponential function for y and z directions
10	1,2	Heaviside function for x direction, Dirac function for y and z directions
11	1,2	Heaviside function for x and z directions, Dirac function for y direction
12	1,2	Heaviside function for x , Dirac function for y , exponential function for z direction
13	1,2	Heaviside function for x and y directions, Dirac function for z direction
14	1,2,3	Heaviside function for x, y and z directions
15	1,2,3	Heaviside function for x and y directions, exponential function for z direction
16	1,2	Heaviside function for x , exponential function for y , Dirac function for z direction
17	1,2,3	Heaviside function for x and z directions, exponential function for y direction
18	1,2,3	Heaviside function for x direction, exponential function for y and z directions
19	1,2	Exponential function for x direction, Dirac function for y and z directions
20	1,2	Exponential function for x , Dirac function for y , Heaviside function for z direction
21	1,2	Exponential function for x and z directions, Dirac function for y direction
22	1,2	Exponential function for x , Heaviside function for y , Dirac function for z direction
23	1,2,3	Exponential function for x direction, Heaviside function for y and z directions
24	1,2,3	Exponential function for x and z directions, Heaviside function for y direction
25	1,2	Exponential function for x and y directions, Dirac function for z direction
26	1,2,3	Exponential function for x and y directions, Heaviside function for z direction
27	1,2,3	Exponential function for x, y and z directions
<i>Circular Geometry</i>		
28	1,2	Dirac function for x direction, Heaviside function for r_c direction
29	1,2	Dirac function for x direction, exponential function for r_c direction
30	1,2,3	Heaviside function for x and r_c directions
31	1,2,3	Heaviside function for x direction, exponential function for r_c direction
32	1,2,3	Exponential function for x direction, Heaviside function for r_c direction
33	1,2,3	Exponential function for x and r_c directions
<i>Spherical Geometry</i>		
34	2,3	Heaviside function for x and r_s directions
35	2,3	Exponential function for x and r_s directions

APPENDIX C. INPUT FILE LISTINGS

ONEA.IN

3 50

Fig. 6: Instantaneous application from disc (cm,d)

20.0	5.0	10.0	2.5	2.5
0.50	0.10	0.0	0.0	
50.0	1.00	1	1	

BVP Dirac for x, Heaviside for r (circular geometry)

28	0	1	1	
0.0	20.0			
0.0	2.5			
0.25	0.0	20.0		
0.0	50.0	50.0		
0.0	0.0	0.0		
0.0	0.0	0.0		

Fig. 6: Instantaneous application from disc (cm,d)

20.0	5.0	10.0	2.5	2.5
0.50	1.00	0.0	0.0	
50.0	1.00	1	1	

BVP Dirac for x, Heaviside for r (circular geometry)

28	0	1	1	
0.0	20.0			
0.0	2.5			
0.25	0.0	20.0		
0.0	50.0	50.0		
0.0	0.0	0.0		
0.0	0.0	0.0		

Fig. 6: Instantaneous application from disc (cm,d)

20.0	5.0	10.0	2.5	2.5
0.50	10.0	0.0	0.0	
50.0	1.00	1	1	

BVP Dirac for x, Heaviside for r (circular geometry)

28	0	1	1	
0.0	20.0			
0.0	2.5			
0.25	0.0	20.0		
0.0	50.0	50.0		
0.0	0.0	0.0		
0.0	0.0	0.0		

ONEB.IN

3 50

Fig. 7: Instantaneous application from disc (cm,d)

20.0	5.0	10.0	2.5	2.5
0.50	0.1	0.0	0.0	
50.0	1.00	1	1	

BVP Dirac for x, Heaviside for r (circular geometry)

28	0	1	1	
0.0	20.0			
0.0	2.5			
6.0	6.0	12.0		
0.0	50.0	50.0		
0.5	0.0	10.0		
0.0	0.0	0.0		

Fig. 7: Instantaneous application from disc (cm,d)

20.0	5.0	10.0	2.5	2.5
0.50	1.0	0.0	0.0	
50.0	1.00	1	1	

BVP Dirac for x, Heaviside for r (circular geometry)

28	0	1	1	
0.0	20.0			
0.0	2.5			
6.0	6.0	12.0		
0.0	50.0	50.0		
0.5	0.0	10.0		
0.0	0.0	0.0		

Fig. 7: Instantaneous application from disc (cm,d)

20.0	5.0	10.0	2.5	2.5
0.50	10.0	0.0	0.0	
50.0	1.00	1	1	
BVP Dirac for x, Heaviside for r (circular geometry)				
28	0	1	1	
0.0	20.0			
0.0	2.5			
6.0	6.0	12.0		
0.0	50.0	50.0		
0.5	0.0	10.0		
0.0	0.0	0.0		

TWOA.IN

1 50

Fig. 8: Heaviside application finite rectangle

20.0	4.0	20.0	10.0	5.0
0.50	0.25	0.0	0.0	
20.0	1.00	1	0	

BVP Dirac for x, Heaviside for y and z

14	1	1	1	
1.0	20.0			
-2.5	2.5			
-2.5	2.5			
5.0	5.0	15.0		
1.0	0.0	20.0		
0.0	0.0	0.0		
0.0	0.0	0.0		

TWOB.IN

1 50

Fig. 9: Heaviside application finite rectangle

20.0	4.0	20.0	10.0	5.0
0.50	0.25	0.0	0.0	
20.0	1.00	1	0	

BVP Dirac for x, Heaviside for y and z

14	1	1	1	
1.0	40.0			
-2.5	2.5			
-2.5	2.5			
0.0	40.0	40.0		
5.0	5.0	10.0		
0.1	0.0	10.0		
0.1	0.0	10.0		

THREE.IN

1 50

Fig. 10: Heaviside initial, finite rectangle

50.0	1.0	20.0	5.0	5.0
0.50	1.00	0.0	0.0	
100.0	1.0	2	0	

IVP Heaviside for x, y and z

14	3	1	1	
5.0	1.0	15.0	0.0	25.0
15.0	25.0			0.5
-100.	100.			35.0
0.0	0.5	0.5		
0.5	0.0	100.0		
0.5	0.0	40.0		
0.0	0.0	0.0		

FOUR.IN

1 20

Fig. 11: Exponential distribution about (5,0,0)

5.0	1.0	10.0	5.0	5.0
0.5	1.0	0.0	0.0	
20.0	1.0	2	0	

IVP, exponential for spherical coordinate

35	0	0	0	
----	---	---	---	--

5.0	1.0	2.0	40.0
0.0	1.0	1.0	
1.0	0.0	40.0	
1.0	0.0	40.0	
0.0	0.0	0.0	

FIVE.IN

1 20

Fig. 12: Heaviside production

5.0	1.0	5.0	2.0	2.0
0.5	5.0	0.5	0.0	
20.0	0.25	3	0	

PVP, Heaviside, circular coordinate

30	1	1	0
0.0	0.5	1.0	10.0
0.0	2.5		
0.0	20.0	20.0	
0.125	0.0	20.0	
0.125	0.0	10.0	
0.0	0.0	0.0	

APPENDIX D. OUTPUT FILE LISTINGS

ONEA.OUT

```
*****
*          *
*          N3DADE          *
*          *
* ANALYTICAL SOLUTIONS FOR NONEQUILIBRIUM SOLUTE TRANSPORT          *
* IN 3-D SEMI-INFINITE POROUS MEDIA          *
*          *
* FLUX-AVERAGED CONCENTRATIONS          *
* Fig. 6: Instantaneous application from disc (cm,d)          *
*****
```

MODEL PARAMETERS

```
=====
```

NAME	VALUE
------	-------

dimensional

V	20.00
R	5.00
Dx	10.00
Dy	2.50
Dz	2.50

dimensionless

BETA	.50
OMEGA	.10
MU1	.00
MU2	.00

CONSTANTS

```
=====
```

L	=	50.00
Co	=	1.00

BOUNDARY VALUE PROBLEM 28

```
=====
```

DIRAC INPUT FUNCTION

t0=	.00	m=	20.00
-----	-----	----	-------

HEAVISIDE DISTRIBUTION FOR CIRCULAR GEOMETRY

i	rin	rend
1	.00	2.50

INDEPENDENT VARIABLES

```
=====
```

VARIABLE	INCREMENT	MINIMUM	MAXIMUM
t	.250	.000	20.000
x	.000	50.000	50.000
y	.000	.000	.000
z	.000	.000	.000

PREDICTED CONCENTRATIONS

```
=====
```

NO	EQUILIBRIUM		NONEQUILIBRIUM		TOTAL		t	x	y	z
	C	C/Co	C	C/Co	C _t	C _t /Co				
1	.000	.000	.000	.000	.000	.000	.00	50.00	.00	.00
2	.000	.000	.000	.000	.000	.000	.25	50.00	.00	.00
3	.000	.000	.000	.000	.000	.000	.50	50.00	.00	.00
4	.000	.000	.000	.000	.000	.000	.75	50.00	.00	.00

5	.000	.000	.000	.000	.000	.000	1.00	50.00	.00	.00
6	.000	.000	.000	.000	.000	.000	1.25	50.00	.00	.00
7	.000	.000	.000	.000	.000	.000	1.50	50.00	.00	.00
8	.000	.000	.000	.000	.000	.000	1.75	50.00	.00	.00
9	.000	.000	.000	.000	.000	.000	2.00	50.00	.00	.00
10	.000	.000	.000	.000	.000	.000	2.25	50.00	.00	.00
11	.000	.000	.000	.000	.000	.000	2.50	50.00	.00	.00
12	.000	.000	.000	.000	.000	.000	2.75	50.00	.00	.00
13	.000	.000	.000	.000	.000	.001	3.00	50.00	.00	.00
14	.000	.000	.000	.000	.001	.001	3.25	50.00	.00	.00
15	.003	.003	.000	.000	.008	.008	3.50	50.00	.00	.00
16	.020	.020	.000	.000	.050	.050	3.75	50.00	.00	.00
17	.085	.085	.000	.000	.212	.212	4.00	50.00	.00	.00
18	.268	.268	.001	.001	.672	.672	4.25	50.00	.00	.00
19	.663	.663	.003	.003	1.664	1.664	4.50	50.00	.00	.00
20	1.331	1.331	.007	.007	3.344	3.344	4.75	50.00	.00	.00
21	2.240	2.240	.014	.014	5.633	5.633	5.00	50.00	.00	.00
22	3.240	3.240	.024	.024	8.162	8.162	5.25	50.00	.00	.00
23	4.116	4.116	.039	.039	10.387	10.387	5.50	50.00	.00	.00
24	4.669	4.669	.057	.057	11.815	11.815	5.75	50.00	.00	.00
25	4.800	4.800	.075	.075	12.188	12.188	6.00	50.00	.00	.00
26	4.525	4.525	.094	.094	11.548	11.548	6.25	50.00	.00	.00
27	3.953	3.953	.111	.111	10.159	10.159	6.50	50.00	.00	.00
28	3.228	3.228	.124	.124	8.380	8.380	6.75	50.00	.00	.00
29	2.482	2.482	.135	.135	6.543	6.543	7.00	50.00	.00	.00
30	1.810	1.810	.143	.143	4.883	4.883	7.25	50.00	.00	.00
31	1.259	1.259	.149	.149	3.519	3.519	7.50	50.00	.00	.00
32	.840	.840	.152	.152	2.481	2.481	7.75	50.00	.00	.00
33	.541	.541	.154	.154	1.739	1.739	8.00	50.00	.00	.00
34	.339	.339	.156	.156	1.236	1.236	8.25	50.00	.00	.00
35	.208	.208	.156	.156	.910	.910	8.50	50.00	.00	.00
36	.127	.127	.156	.156	.706	.706	8.75	50.00	.00	.00
37	.078	.078	.156	.156	.584	.584	9.00	50.00	.00	.00
38	.050	.050	.155	.155	.512	.512	9.25	50.00	.00	.00
39	.034	.034	.155	.155	.471	.471	9.50	50.00	.00	.00
40	.025	.025	.155	.155	.448	.448	9.75	50.00	.00	.00
41	.020	.020	.154	.154	.435	.435	10.00	50.00	.00	.00
42	.018	.018	.153	.153	.427	.427	10.25	50.00	.00	.00
43	.016	.016	.153	.153	.423	.423	10.50	50.00	.00	.00
44	.016	.016	.152	.152	.420	.420	10.75	50.00	.00	.00
45	.015	.015	.152	.152	.417	.417	11.00	50.00	.00	.00
46	.015	.015	.151	.151	.415	.415	11.25	50.00	.00	.00
47	.015	.015	.151	.151	.414	.414	11.50	50.00	.00	.00
48	.015	.015	.150	.150	.412	.412	11.75	50.00	.00	.00
49	.015	.015	.150	.150	.411	.411	12.00	50.00	.00	.00
50	.015	.015	.149	.149	.409	.409	12.25	50.00	.00	.00
51	.015	.015	.149	.149	.408	.408	12.50	50.00	.00	.00
52	.014	.014	.148	.148	.406	.406	12.75	50.00	.00	.00
53	.014	.014	.147	.147	.405	.405	13.00	50.00	.00	.00
54	.014	.014	.147	.147	.403	.403	13.25	50.00	.00	.00
55	.014	.014	.146	.146	.402	.402	13.50	50.00	.00	.00
56	.014	.014	.146	.146	.400	.400	13.75	50.00	.00	.00
57	.014	.014	.145	.145	.399	.399	14.00	50.00	.00	.00
58	.014	.014	.145	.145	.397	.397	14.25	50.00	.00	.00
59	.014	.014	.144	.144	.396	.396	14.50	50.00	.00	.00
60	.014	.014	.144	.144	.395	.395	14.75	50.00	.00	.00
61	.014	.014	.143	.143	.393	.393	15.00	50.00	.00	.00
62	.014	.014	.143	.143	.392	.392	15.25	50.00	.00	.00
63	.014	.014	.142	.142	.390	.390	15.50	50.00	.00	.00
64	.014	.014	.142	.142	.389	.389	15.75	50.00	.00	.00
65	.014	.014	.141	.141	.387	.387	16.00	50.00	.00	.00
66	.014	.014	.141	.141	.386	.386	16.25	50.00	.00	.00
67	.014	.014	.140	.140	.385	.385	16.50	50.00	.00	.00
68	.014	.014	.140	.140	.383	.383	16.75	50.00	.00	.00
69	.014	.014	.139	.139	.382	.382	17.00	50.00	.00	.00
70	.014	.014	.139	.139	.381	.381	17.25	50.00	.00	.00
71	.013	.013	.138	.138	.379	.379	17.50	50.00	.00	.00
72	.013	.013	.138	.138	.378	.378	17.75	50.00	.00	.00
73	.013	.013	.137	.137	.376	.376	18.00	50.00	.00	.00
74	.013	.013	.137	.137	.375	.375	18.25	50.00	.00	.00

	EQUILIBRIUM	NONEQUILIBRIUM	TOTAL								
NO	C	C/Co	C	C/Co	C _t	C _t /C ₀	t	x	y	z	
1	.000	.000	.000	.000	.000	.000	.00	50.00	.00	.00	

```
*****
*          *
*          *          N3DADE          *
*          *          *
*          *          ANALYTICAL SOLUTIONS FOR NONEQUILIBRIUM SOLUTE TRANSPORT          *
*          *          IN 3-D SEMI-INFINITE POROUS MEDIA          *
*          *          *
*          *          FLUX-AVERAGED CONCENTRATIONS          *
*          *          Fig. 6: Instantaneous application from disc (cm,d)          *
*          *          *
*****
```

MODEL PARAMETERS

=====

NAME	VALUE
------	-------

dimensional

V	20.00
R	5.00
Dx	10.00
Dy	2.50
Dz	2.50

dimensionless

BETA	.50
OMEGA	1.00
MU1	.00
MU2	.00

CONSTANTS

=====

L =	50.00
Co =	1.00

BOUNDARY VALUE PROBLEM 28

=====

DIRAC INPUT FUNCTION

t0=	.00	m=	20.00
-----	-----	----	-------

HEAVISIDE DISTRIBUTION FOR CIRCULAR GEOMETRY

i	r _{in}	r _{end}
1	.00	2.50

INDEPENDENT VARIABLES

=====

VARIABLE	INCREMENT	MINIMUM	MAXIMUM
t	.250	.000	20.000
x	.000	50.000	50.000
y	.000	.000	.000
z	.000	.000	.000

PREDICTED CONCENTRATIONS

=====

	EQUILIBRIUM	NONEQUILIBRIUM	TOTAL								
NO	C	C/Co	C	C/Co	C _t	C _t /C ₀	t	x	y	z	
1	.000	.000	.000	.000	.000	.000	.00	50.00	.00	.00	

..

ONEB.OUT

```
*****
*          N3DADE
*
*      ANALYTICAL SOLUTIONS FOR NONEQUILIBRIUM SOLUTE TRANSPORT
*      IN 3-D SEMI-INFINITE POROUS MEDIA
*
*      FLUX-AVERAGED CONCENTRATIONS
*      Fig. 7: Instantaneous application from disc (cm,d)
*****
*****
```

MODEL PARAMETERS

```
=====
```

NAME	VALUE
------	-------

dimensional

V	20.00
R	5.00
Dx	10.00
Dy	2.50
Dz	2.50

dimensionless

BETA	.50
OMEGA	.10
MU1	.00
MU2	.00

CONSTANTS

```
=====
```

L	=	50.00
Co	=	1.00

BOUNDARY VALUE PROBLEM 28

```
=====
```

DIRAC INPUT FUNCTION

t0=	.00	m=	20.00
-----	-----	----	-------

HEAVISIDE DISTRIBUTION FOR CIRCULAR GEOMETRY

i	rin	rend
1	.00	2.50

INDEPENDENT VARIABLES

```
=====
```

VARIABLE	INCREMENT	MINIMUM	MAXIMUM
t	6.000	6.000	12.000
x	.000	50.000	50.000
y	.500	.000	10.000
z	.000	.000	.000

PREDICTED CONCENTRATIONS

```
=====
```

NO	EQUILIBRIUM		NONEQUILIBRIUM		TOTAL		t	x	y	z
	C	C/Co	C	C/Co	C _t	C _t /Co				
1	4.800	4.800	.075	.075	12.188	12.188	6.00	50.00	.00	.00
2	4.756	4.756	.075	.075	12.078	12.078	6.00	50.00	.50	.00
3	4.628	4.628	.073	.073	11.751	11.751	6.00	50.00	1.00	.00
4	4.422	4.422	.069	.069	11.226	11.226	6.00	50.00	1.50	.00
5	4.148	4.148	.064	.064	10.530	10.530	6.00	50.00	2.00	.00
6	3.821	3.821	.059	.059	9.698	9.698	6.00	50.00	2.50	.00
7	3.455	3.455	.053	.053	8.770	8.770	6.00	50.00	3.00	.00

8	3.068	3.068	.046	.046	7.786	7.786	6.00	50.00	3.50	.00
9	2.675	2.675	.040	.040	6.786	6.786	6.00	50.00	4.00	.00
10	2.289	2.289	.034	.034	5.806	5.806	6.00	50.00	4.50	.00
11	1.923	1.923	.028	.028	4.877	4.877	6.00	50.00	5.00	.00
12	1.586	1.586	.022	.022	4.021	4.021	6.00	50.00	5.50	.00
13	1.284	1.284	.018	.018	3.255	3.255	6.00	50.00	6.00	.00
14	1.020	1.020	.014	.014	2.585	2.585	6.00	50.00	6.50	.00
15	.796	.796	.011	.011	2.016	2.016	6.00	50.00	7.00	.00
16	.609	.609	.008	.008	1.542	1.542	6.00	50.00	7.50	.00
17	.457	.457	.006	.006	1.158	1.158	6.00	50.00	8.00	.00
18	.337	.337	.004	.004	.853	.853	6.00	50.00	8.50	.00
19	.244	.244	.003	.003	.617	.617	6.00	50.00	9.00	.00
20	.173	.173	.002	.002	.438	.438	6.00	50.00	9.50	.00
21	.120	.120	.001	.001	.305	.305	6.00	50.00	10.00	.00
22	.015	.015	.150	.150	.411	.411	12.00	50.00	.00	.00
23	.015	.015	.148	.148	.407	.407	12.00	50.00	.50	.00
24	.014	.014	.144	.144	.396	.396	12.00	50.00	1.00	.00
25	.014	.014	.138	.138	.379	.379	12.00	50.00	1.50	.00
26	.013	.013	.129	.129	.355	.355	12.00	50.00	2.00	.00
27	.012	.012	.119	.119	.328	.328	12.00	50.00	2.50	.00
28	.011	.011	.108	.108	.297	.297	12.00	50.00	3.00	.00
29	.009	.009	.096	.096	.264	.264	12.00	50.00	3.50	.00
30	.008	.008	.084	.084	.230	.230	12.00	50.00	4.00	.00
31	.007	.007	.072	.072	.198	.198	12.00	50.00	4.50	.00
32	.006	.006	.061	.061	.167	.167	12.00	50.00	5.00	.00
33	.005	.005	.050	.050	.138	.138	12.00	50.00	5.50	.00
34	.004	.004	.041	.041	.112	.112	12.00	50.00	6.00	.00
35	.003	.003	.033	.033	.090	.090	12.00	50.00	6.50	.00
36	.003	.003	.026	.026	.071	.071	12.00	50.00	7.00	.00
37	.002	.002	.020	.020	.055	.055	12.00	50.00	7.50	.00
38	.002	.002	.015	.015	.041	.041	12.00	50.00	8.00	.00
39	.001	.001	.011	.011	.031	.031	12.00	50.00	8.50	.00
40	.001	.001	.008	.008	.023	.023	12.00	50.00	9.00	.00
41	.001	.001	.006	.006	.016	.016	12.00	50.00	9.50	.00
42	.000	.000	.004	.004	.012	.012	12.00	50.00	10.00	.00

```
*****
*          N3DADE
*
* ANALYTICAL SOLUTIONS FOR NONEQUILIBRIUM SOLUTE TRANSPORT
* IN 3-D SEMI-INFINITE POROUS MEDIA
*
* FLUX-AVERAGED CONCENTRATIONS
* Fig. 7: Instantaneous application from disc (cm,d)
*
```

MODEL PARAMETERS

=====

NAME	VALUE
dimensional	
V	20.00
R	5.00
Dx	10.00
Dy	2.50
Dz	2.50

dimensionless

BETA	.50
OMEGA	1.00
MU1	.00
MU2	.00
..	
..	

TWOA.OUT

```
*****
*          N3DADE
*
*      ANALYTICAL SOLUTIONS FOR NONEQUILIBRIUM SOLUTE TRANSPORT
*      IN 3-D SEMI-INFINITE POROUS MEDIA
*
*      VOLUME-AVERAGED CONCENTRATIONS
*      Fig. 8: Heaviside application finite rectangle
*****
*****
```

MODEL PARAMETERS

```
=====
```

NAME	VALUE
------	-------

dimensional

V	20.00
R	4.00
Dx	20.00
Dy	10.00
Dz	5.00

dimensionless

BETA	.50
OMEGA	.25
MU1	.00
MU2	.00

CONSTANTS

```
=====
```

L	= 20.00
Co	= 1.00

BOUNDARY VALUE PROBLEM 14

```
=====
```

HEAVISIDE INPUT FUNCTION

i	g	tin	tend
1	1.00	.00	20.00

HEAVISIDE DISTRIBUTION FOR Y-DIRECTION

i	yin	yend
1	-2.50	2.50

HEAVISIDE DISTRIBUTION FOR Z-DIRECTION

i	zin	zend
1	-2.50	2.50

INDEPENDENT VARIABLES

```
=====
```

VARIABLE	INCREMENT	MINIMUM	MAXIMUM
t	5.000	5.000	15.000
x	1.000	.000	20.000
y	.000	.000	.000
z	.000	.000	.000

PREDICTED CONCENTRATIONS

```
=====
```

NO	EQUILIBRIUM		NONEQUILIBRIUM		TOTAL		t	x	y	z
	C	C/Co	C	C/Co	C _t	C _t /Co				
1	.948	.948	.435	.435	2.764	2.764	5.00	.00	.00	.00

2	.892	.892	.403	.403	2.589	2.589	5.00	1.00	.00	.00
3	.820	.820	.366	.366	2.372	2.372	5.00	2.00	.00	.00
4	.747	.747	.328	.328	2.151	2.151	5.00	3.00	.00	.00
5	.678	.678	.293	.293	1.943	1.943	5.00	4.00	.00	.00
6	.615	.615	.262	.262	1.754	1.754	5.00	5.00	.00	.00
7	.559	.559	.234	.234	1.587	1.587	5.00	6.00	.00	.00
8	.510	.510	.210	.210	1.441	1.441	5.00	7.00	.00	.00
9	.468	.468	.189	.189	1.313	1.313	5.00	8.00	.00	.00
10	.430	.430	.171	.171	1.202	1.202	5.00	9.00	.00	.00
11	.397	.397	.154	.154	1.103	1.103	5.00	10.00	.00	.00
12	.368	.368	.140	.140	1.017	1.017	5.00	11.00	.00	.00
13	.342	.342	.128	.128	.940	.940	5.00	12.00	.00	.00
14	.319	.319	.117	.117	.872	.872	5.00	13.00	.00	.00
15	.299	.299	.107	.107	.811	.811	5.00	14.00	.00	.00
16	.280	.280	.098	.098	.756	.756	5.00	15.00	.00	.00
17	.263	.263	.090	.090	.706	.706	5.00	16.00	.00	.00
18	.248	.248	.083	.083	.661	.661	5.00	17.00	.00	.00
19	.234	.234	.076	.076	.621	.621	5.00	18.00	.00	.00
20	.221	.221	.070	.070	.583	.583	5.00	19.00	.00	.00
21	.210	.210	.065	.065	.549	.549	5.00	20.00	.00	.00
22	.948	.948	.672	.672	3.241	3.241	10.00	.00	.00	.00
23	.901	.901	.635	.635	3.072	3.072	10.00	1.00	.00	.00
24	.826	.826	.578	.578	2.808	2.808	10.00	2.00	.00	.00
25	.756	.756	.525	.525	2.562	2.562	10.00	3.00	.00	.00
26	.688	.688	.475	.475	2.324	2.324	10.00	4.00	.00	.00
27	.626	.626	.429	.429	2.109	2.109	10.00	5.00	.00	.00
28	.571	.571	.388	.388	1.918	1.918	10.00	6.00	.00	.00
29	.522	.522	.353	.353	1.751	1.751	10.00	7.00	.00	.00
30	.480	.480	.322	.322	1.604	1.604	10.00	8.00	.00	.00
31	.443	.443	.295	.295	1.477	1.477	10.00	9.00	.00	.00
32	.411	.411	.271	.271	1.364	1.364	10.00	10.00	.00	.00
33	.382	.382	.250	.250	1.264	1.264	10.00	11.00	.00	.00
34	.357	.357	.231	.231	1.176	1.176	10.00	12.00	.00	.00
35	.334	.334	.215	.215	1.098	1.098	10.00	13.00	.00	.00
36	.314	.314	.200	.200	1.027	1.027	10.00	14.00	.00	.00
37	.295	.295	.187	.187	.964	.964	10.00	15.00	.00	.00
38	.279	.279	.175	.175	.907	.907	10.00	16.00	.00	.00
39	.264	.264	.164	.164	.855	.855	10.00	17.00	.00	.00
40	.250	.250	.154	.154	.808	.808	10.00	18.00	.00	.00
41	.237	.237	.145	.145	.765	.765	10.00	19.00	.00	.00
42	.226	.226	.137	.137	.725	.725	10.00	20.00	.00	.00
43	.947	.947	.799	.799	3.493	3.493	15.00	.00	.00	.00
44	.895	.895	.752	.752	3.293	3.293	15.00	1.00	.00	.00
45	.829	.829	.694	.694	3.046	3.046	15.00	2.00	.00	.00
46	.760	.760	.634	.634	2.789	2.789	15.00	3.00	.00	.00
47	.693	.693	.575	.575	2.535	2.535	15.00	4.00	.00	.00
48	.631	.631	.522	.522	2.307	2.307	15.00	5.00	.00	.00
49	.577	.577	.475	.475	2.104	2.104	15.00	6.00	.00	.00
50	.529	.529	.434	.434	1.925	1.925	15.00	7.00	.00	.00
51	.487	.487	.397	.397	1.769	1.769	15.00	8.00	.00	.00
52	.451	.451	.366	.366	1.633	1.633	15.00	9.00	.00	.00
53	.418	.418	.338	.338	1.513	1.513	15.00	10.00	.00	.00
54	.390	.390	.314	.314	1.407	1.407	15.00	11.00	.00	.00
55	.365	.365	.292	.292	1.313	1.313	15.00	12.00	.00	.00
56	.342	.342	.273	.273	1.229	1.229	15.00	13.00	.00	.00
57	.322	.322	.255	.255	1.154	1.154	15.00	14.00	.00	.00
58	.304	.304	.240	.240	1.087	1.087	15.00	15.00	.00	.00
59	.287	.287	.226	.226	1.026	1.026	15.00	16.00	.00	.00
60	.273	.273	.213	.213	.971	.971	15.00	17.00	.00	.00
61	.259	.259	.201	.201	.920	.920	15.00	18.00	.00	.00
62	.247	.247	.190	.190	.874	.874	15.00	19.00	.00	.00
63	.235	.235	.181	.181	.832	.832	15.00	20.00	.00	.00

TWOB.OUT

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*****
*          N3DADE
*
*      ANALYTICAL SOLUTIONS FOR NONEQUILIBRIUM SOLUTE TRANSPORT
*      IN 3-D SEMI-INFINITE POROUS MEDIA
*
*      VOLUME-AVERAGED CONCENTRATIONS
*      Fig. 9: Heaviside application finite rectangle
*****
*****
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MODEL PARAMETERS

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NAME	VALUE
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dimensional

V	20.00
R	4.00
Dx	20.00
Dy	10.00
Dz	5.00

dimensionless

BETA	.50
OMEGA	.25
MU1	.00
MU2	.00

CONSTANTS

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=====
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L	= 20.00
Co	= 1.00

BOUNDARY VALUE PROBLEM 14

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=====
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HEAVISIDE INPUT FUNCTION

i	g	tin	tend
1	1.00	.00	40.00

HEAVISIDE DISTRIBUTION FOR Y-DIRECTION

i	yin	yend
1	-2.50	2.50

HEAVISIDE DISTRIBUTION FOR Z-DIRECTION

i	zin	zend
1	-2.50	2.50

INDEPENDENT VARIABLES

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=====
```

VARIABLE	INCREMENT	MINIMUM	MAXIMUM
t	.000	40.000	40.000
x	5.000	5.000	10.000
y	.100	.000	10.000
z	.100	.000	10.000

PREDICTED CONCENTRATIONS

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=====
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NO	EQUILIBRIUM		NONEQUILIBRIUM		TOTAL		t	x	y	z
	C	C/Co	C	C/Co	C _t	C _t /Co				
1	.639	.639	.634	.634	2.546	2.546	40.00	5.00	.00	.00
2	.639	.639	.633	.633	2.544	2.544	40.00	5.00	.00	.10
3	.638	.638	.632	.632	2.539	2.539	40.00	5.00	.00	.20

4	.635	.635	.630	.630	2.530	2.530	40.00	5.00	.00	.30
5	.632	.632	.626	.626	2.517	2.517	40.00	5.00	.00	.40
6	.628	.628	.622	.622	2.501	2.501	40.00	5.00	.00	.50
7	.623	.623	.617	.617	2.481	2.481	40.00	5.00	.00	.60
8	.617	.617	.612	.612	2.458	2.458	40.00	5.00	.00	.70
9	.610	.610	.605	.605	2.430	2.430	40.00	5.00	.00	.80
10	.602	.602	.597	.597	2.399	2.399	40.00	5.00	.00	.90
11	.594	.594	.588	.588	2.364	2.364	40.00	5.00	.00	1.00
12	.584	.584	.579	.579	2.325	2.325	40.00	5.00	.00	1.10
13	.573	.573	.568	.568	2.282	2.282	40.00	5.00	.00	1.20
14	.561	.561	.556	.556	2.236	2.236	40.00	5.00	.00	1.30
15	.549	.549	.544	.544	2.185	2.185	40.00	5.00	.00	1.40
16	.535	.535	.530	.530	2.131	2.131	40.00	5.00	.00	1.50
17	.521	.521	.516	.516	2.073	2.073	40.00	5.00	.00	1.60
18	.505	.505	.501	.501	2.012	2.012	40.00	5.00	.00	1.70
19	.489	.489	.485	.485	1.948	1.948	40.00	5.00	.00	1.80
20	.472	.472	.468	.468	1.881	1.881	40.00	5.00	.00	1.90
21	.455	.455	.451	.451	1.811	1.811	40.00	5.00	.00	2.00
22	.437	.437	.433	.433	1.739	1.739	40.00	5.00	.00	2.10
23	.418	.418	.414	.414	1.665	1.665	40.00	5.00	.00	2.20
24	.399	.399	.396	.396	1.589	1.589	40.00	5.00	.00	2.30
25	.380	.380	.376	.376	1.513	1.513	40.00	5.00	.00	2.40
26	.361	.361	.357	.357	1.436	1.436	40.00	5.00	.00	2.50
27	.341	.341	.338	.338	1.358	1.358	40.00	5.00	.00	2.60
28	.322	.322	.319	.319	1.281	1.281	40.00	5.00	.00	2.70
29	.303	.303	.300	.300	1.205	1.205	40.00	5.00	.00	2.80
30	.284	.284	.281	.281	1.130	1.130	40.00	5.00	.00	2.90
31	.265	.265	.263	.263	1.057	1.057	40.00	5.00	.00	3.00
32	.247	.247	.245	.245	.985	.985	40.00	5.00	.00	3.10
33	.230	.230	.228	.228	.916	.916	40.00	5.00	.00	3.20
34	.213	.213	.211	.211	.850	.850	40.00	5.00	.00	3.30
35	.197	.197	.195	.195	.786	.786	40.00	5.00	.00	3.40
36	.182	.182	.180	.180	.725	.725	40.00	5.00	.00	3.50
37	.168	.168	.166	.166	.667	.667	40.00	5.00	.00	3.60
38	.154	.154	.152	.152	.613	.613	40.00	5.00	.00	3.70
39	.141	.141	.140	.140	.561	.561	40.00	5.00	.00	3.80
40	.129	.129	.128	.128	.513	.513	40.00	5.00	.00	3.90
41	.118	.118	.116	.116	.468	.468	40.00	5.00	.00	4.00
42	.107	.107	.106	.106	.427	.427	40.00	5.00	.00	4.10
43	.097	.097	.096	.096	.388	.388	40.00	5.00	.00	4.20
44	.088	.088	.088	.088	.352	.352	40.00	5.00	.00	4.30
45	.080	.080	.079	.079	.319	.319	40.00	5.00	.00	4.40
46	.073	.073	.072	.072	.289	.289	40.00	5.00	.00	4.50
47	.066	.066	.065	.065	.261	.261	40.00	5.00	.00	4.60
48	.059	.059	.059	.059	.236	.236	40.00	5.00	.00	4.70
49	.054	.054	.053	.053	.213	.213	40.00	5.00	.00	4.80
50	.048	.048	.048	.048	.192	.192	40.00	5.00	.00	4.90
51	.043	.043	.043	.043	.173	.173	40.00	5.00	.00	5.00
52	.039	.039	.039	.039	.156	.156	40.00	5.00	.00	5.10
53	.035	.035	.035	.035	.140	.140	40.00	5.00	.00	5.20
54	.032	.032	.031	.031	.126	.126	40.00	5.00	.00	5.30
55	.028	.028	.028	.028	.113	.113	40.00	5.00	.00	5.40
56	.025	.025	.025	.025	.101	.101	40.00	5.00	.00	5.50
57	.023	.023	.023	.023	.091	.091	40.00	5.00	.00	5.60
58	.020	.020	.020	.020	.081	.081	40.00	5.00	.00	5.70
59	.018	.018	.018	.018	.073	.073	40.00	5.00	.00	5.80
60	.016	.016	.016	.016	.065	.065	40.00	5.00	.00	5.90
61	.015	.015	.015	.015	.058	.058	40.00	5.00	.00	6.00
62	.013	.013	.013	.013	.052	.052	40.00	5.00	.00	6.10
63	.012	.012	.012	.012	.047	.047	40.00	5.00	.00	6.20
64	.011	.011	.010	.010	.042	.042	40.00	5.00	.00	6.30
65	.009	.009	.009	.009	.037	.037	40.00	5.00	.00	6.40
66	.008	.008	.008	.008	.033	.033	40.00	5.00	.00	6.50
67	.008	.008	.007	.007	.030	.030	40.00	5.00	.00	6.60
68	.007	.007	.007	.007	.027	.027	40.00	5.00	.00	6.70
69	.006	.006	.006	.006	.024	.024	40.00	5.00	.00	6.80
70	.005	.005	.005	.005	.021	.021	40.00	5.00	.00	6.90

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THREE.OUT

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*****
*          N3DADE
*
* ANALYTICAL SOLUTIONS FOR NONEQUILIBRIUM SOLUTE TRANSPORT
* IN 3-D SEMI-INFINITE POROUS MEDIA
*
* VOLUME-AVERAGED CONCENTRATIONS
* Fig. 10: Heaviside initial, finite rectangle
*****
*****
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MODEL PARAMETERS

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NAME	VALUE
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dimensional

V	50.00
R	1.00
Dx	20.00
Dy	5.00
Dz	5.00

dimensionless

BETA	.50
OMEGA	1.00
MU1	.00
MU2	.00

CONSTANTS

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L = 100.00

Co = 1.00

INITIAL VALUE PROBLEM 14

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HEAVISIDE INITIAL DISTRIBUTION

i	f	xin	xend
1	1.00	5.00	15.00
2	.00	15.00	25.00
3	.50	25.00	35.00

HEAVISIDE DISTRIBUTION FOR Y-DIRECTION

i	yin	yend
1	15.00	25.00

HEAVISIDE DISTRIBUTION FOR Z-DIRECTION

i	zin	zend
1	-100.00	100.00

INDEPENDENT VARIABLES

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VARIABLE	INCREMENT	MINIMUM	MAXIMUM
t	.000	.500	.500
x	.500	.000	100.000
y	.500	.000	40.000
z	.000	.000	.000

PREDICTED CONCENTRATIONS

=====

NO	EQUILIBRIUM		NONEQUILIBRIUM		TOTAL		t	x	y	z
	C	C/Co	C	C/Co	Ct	Ct/Co				
1	.000	.000	.000	.000	.000	.000	.50	.00	.00	.00
2	.000	.000	.000	.000	.000	.000	.50	.00	.50	.00
3	.000	.000	.000	.000	.000	.000	.50	.00	1.00	.00
4	.000	.000	.000	.000	.000	.000	.50	.00	1.50	.00
5	.000	.000	.000	.000	.000	.000	.50	.00	2.00	.00
6	.000	.000	.000	.000	.000	.000	.50	.00	2.50	.00
7	.000	.000	.000	.000	.000	.000	.50	.00	3.00	.00
8	.000	.000	.000	.000	.000	.000	.50	.00	3.50	.00
9	.000	.000	.000	.000	.000	.000	.50	.00	4.00	.00
10	.000	.000	.000	.000	.000	.000	.50	.00	4.50	.00
11	.000	.000	.000	.000	.000	.000	.50	.00	5.00	.00
12	.000	.000	.000	.000	.000	.000	.50	.00	5.50	.00
13	.000	.000	.000	.000	.000	.000	.50	.00	6.00	.00
14	.000	.000	.000	.000	.000	.000	.50	.00	6.50	.00
15	.000	.000	.000	.000	.000	.000	.50	.00	7.00	.00
16	.000	.000	.000	.000	.000	.000	.50	.00	7.50	.00
17	.000	.000	.000	.000	.000	.000	.50	.00	8.00	.00
18	.000	.000	.000	.000	.000	.000	.50	.00	8.50	.00
19	.000	.000	.000	.000	.000	.000	.50	.00	9.00	.00
20	.000	.000	.000	.000	.000	.000	.50	.00	9.50	.00
21	.000	.000	.000	.000	.000	.000	.50	.00	10.00	.00
22	.000	.000	.000	.000	.000	.000	.50	.00	10.50	.00
23	.000	.000	.000	.000	.000	.000	.50	.00	11.00	.00
24	.000	.000	.000	.000	.000	.000	.50	.00	11.50	.00
25	.000	.000	.000	.000	.000	.000	.50	.00	12.00	.00
26	.000	.000	.000	.000	.000	.000	.50	.00	12.50	.00
27	.000	.000	.000	.000	.000	.000	.50	.00	13.00	.00
28	.000	.000	.000	.000	.000	.000	.50	.00	13.50	.00
29	.000	.000	.000	.000	.000	.000	.50	.00	14.00	.00
30	.000	.000	.000	.000	.000	.000	.50	.00	14.50	.00
31	.000	.000	.000	.000	.000	.000	.50	.00	15.00	.00
32	.000	.000	.000	.000	.000	.000	.50	.00	15.50	.00
33	.000	.000	.000	.000	.000	.000	.50	.00	16.00	.00
34	.000	.000	.000	.000	.000	.000	.50	.00	16.50	.00
35	.000	.000	.000	.000	.000	.000	.50	.00	17.00	.00
36	.000	.000	.000	.000	.000	.000	.50	.00	17.50	.00
37	.000	.000	.000	.000	.000	.000	.50	.00	18.00	.00
38	.000	.000	.000	.000	.000	.000	.50	.00	18.50	.00
39	.000	.000	.000	.000	.000	.000	.50	.00	19.00	.00
40	.000	.000	.000	.000	.000	.000	.50	.00	19.50	.00
41	.000	.000	.000	.000	.000	.000	.50	.00	20.00	.00
42	.000	.000	.000	.000	.000	.000	.50	.00	20.50	.00
43	.000	.000	.000	.000	.000	.000	.50	.00	21.00	.00
44	.000	.000	.000	.000	.000	.000	.50	.00	21.50	.00
45	.000	.000	.000	.000	.000	.000	.50	.00	22.00	.00
46	.000	.000	.000	.000	.000	.000	.50	.00	22.50	.00
47	.000	.000	.000	.000	.000	.000	.50	.00	23.00	.00
48	.000	.000	.000	.000	.000	.000	.50	.00	23.50	.00
49	.000	.000	.000	.000	.000	.000	.50	.00	24.00	.00
50	.000	.000	.000	.000	.000	.000	.50	.00	24.50	.00
51	.000	.000	.000	.000	.000	.000	.50	.00	25.00	.00
52	.000	.000	.000	.000	.000	.000	.50	.00	25.50	.00
53	.000	.000	.000	.000	.000	.000	.50	.00	26.00	.00
54	.000	.000	.000	.000	.000	.000	.50	.00	26.50	.00
55	.000	.000	.000	.000	.000	.000	.50	.00	27.00	.00
56	.000	.000	.000	.000	.000	.000	.50	.00	27.50	.00
57	.000	.000	.000	.000	.000	.000	.50	.00	28.00	.00
58	.000	.000	.000	.000	.000	.000	.50	.00	28.50	.00
59	.000	.000	.000	.000	.000	.000	.50	.00	29.00	.00
60	.000	.000	.000	.000	.000	.000	.50	.00	29.50	.00
61	.000	.000	.000	.000	.000	.000	.50	.00	30.00	.00
62	.000	.000	.000	.000	.000	.000	.50	.00	30.50	.00
63	.000	.000	.000	.000	.000	.000	.50	.00	31.00	.00
64	.000	.000	.000	.000	.000	.000	.50	.00	31.50	.00

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FOUR.OUT

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*****
*          N3DADE
*
* ANALYTICAL SOLUTIONS FOR NONEQUILIBRIUM SOLUTE TRANSPORT
* IN 3-D SEMI-INFINITE POROUS MEDIA
*
* VOLUME-AVERAGED CONCENTRATIONS
* Fig. 11: Exponential distribution about (5,0,0)
*****

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MODEL PARAMETERS

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NAME	VALUE
------	-------

dimensional

V	5.00
R	1.00
Dx	10.00
Dy	5.00
Dz	5.00

dimensionless

BETA	.50
OMEGA	1.00
MU1	.00
MU2	.00

CONSTANTS

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=====

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L =	20.00
Co =	1.00

INITIAL VALUE PROBLEM 35

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=====

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EXPONENTIAL INITIAL DISTRIBUTION FOR SPHERICAL GEOMETRY x0= 5.00
 fe= 1.00 alpha= 2.00

INDEPENDENT VARIABLES

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=====

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VARIABLE	INCREMENT	MINIMUM	MAXIMUM
t	.000	1.000	1.000
x	1.000	.000	40.000
y	1.000	.000	40.000
z	.000	.000	.000

PREDICTED CONCENTRATIONS

```
=====

```

NO	EQUILIBRIUM		NONEQUILIBRIUM		TOTAL		t	x	y	z
	C	C/Co	C	C/Co	C _t	C _t /Co				
1	.043	.043	.406	.406	.224	.224	1.00	.00	.00	.00
2	.042	.042	.402	.402	.222	.222	1.00	.00	1.00	.00
3	.041	.041	.391	.391	.216	.216	1.00	.00	2.00	.00
4	.040	.040	.374	.374	.207	.207	1.00	.00	3.00	.00
5	.038	.038	.354	.354	.196	.196	1.00	.00	4.00	.00
6	.036	.036	.331	.331	.183	.183	1.00	.00	5.00	.00
7	.034	.034	.307	.307	.170	.170	1.00	.00	6.00	.00
8	.031	.031	.284	.284	.158	.158	1.00	.00	7.00	.00

9	.029	.029	.261	.261	.145	.145	1.00	.00	8.00	.00
10	.027	.027	.240	.240	.133	.133	1.00	.00	9.00	.00
11	.024	.024	.219	.219	.122	.122	1.00	.00	10.00	.00
12	.022	.022	.200	.200	.111	.111	1.00	.00	11.00	.00
13	.020	.020	.183	.183	.102	.102	1.00	.00	12.00	.00
14	.019	.019	.167	.167	.093	.093	1.00	.00	13.00	.00
15	.017	.017	.152	.152	.084	.084	1.00	.00	14.00	.00
16	.016	.016	.138	.138	.077	.077	1.00	.00	15.00	.00
17	.014	.014	.125	.125	.070	.070	1.00	.00	16.00	.00
18	.013	.013	.114	.114	.063	.063	1.00	.00	17.00	.00
19	.012	.012	.104	.104	.058	.058	1.00	.00	18.00	.00
20	.011	.011	.094	.094	.052	.052	1.00	.00	19.00	.00
21	.010	.010	.085	.085	.047	.047	1.00	.00	20.00	.00
22	.009	.009	.077	.077	.043	.043	1.00	.00	21.00	.00
23	.008	.008	.070	.070	.039	.039	1.00	.00	22.00	.00
24	.007	.007	.064	.064	.035	.035	1.00	.00	23.00	.00
25	.007	.007	.058	.058	.032	.032	1.00	.00	24.00	.00
26	.006	.006	.052	.052	.029	.029	1.00	.00	25.00	.00
27	.005	.005	.047	.047	.026	.026	1.00	.00	26.00	.00
28	.005	.005	.043	.043	.024	.024	1.00	.00	27.00	.00
29	.004	.004	.039	.039	.022	.022	1.00	.00	28.00	.00
30	.004	.004	.035	.035	.020	.020	1.00	.00	29.00	.00
31	.004	.004	.032	.032	.018	.018	1.00	.00	30.00	.00
32	.003	.003	.029	.029	.016	.016	1.00	.00	31.00	.00
33	.003	.003	.026	.026	.015	.015	1.00	.00	32.00	.00
34	.003	.003	.024	.024	.013	.013	1.00	.00	33.00	.00
35	.002	.002	.022	.022	.012	.012	1.00	.00	34.00	.00
36	.002	.002	.020	.020	.011	.011	1.00	.00	35.00	.00
37	.002	.002	.018	.018	.010	.010	1.00	.00	36.00	.00
38	.002	.002	.016	.016	.009	.009	1.00	.00	37.00	.00
39	.002	.002	.015	.015	.008	.008	1.00	.00	38.00	.00
40	.001	.001	.013	.013	.007	.007	1.00	.00	39.00	.00
41	.001	.001	.012	.012	.007	.007	1.00	.00	40.00	.00
42	.065	.065	.465	.465	.265	.265	1.00	1.00	.00	.00
43	.065	.065	.460	.460	.262	.262	1.00	1.00	1.00	.00
44	.064	.064	.445	.445	.254	.254	1.00	1.00	2.00	.00
45	.061	.061	.422	.422	.242	.242	1.00	1.00	3.00	.00
46	.058	.058	.396	.396	.227	.227	1.00	1.00	4.00	.00
47	.055	.055	.368	.368	.212	.212	1.00	1.00	5.00	.00
48	.052	.052	.340	.340	.196	.196	1.00	1.00	6.00	.00
49	.048	.048	.312	.312	.180	.180	1.00	1.00	7.00	.00
50	.044	.044	.286	.286	.165	.165	1.00	1.00	8.00	.00
51	.041	.041	.262	.262	.151	.151	1.00	1.00	9.00	.00
52	.038	.038	.239	.239	.138	.138	1.00	1.00	10.00	.00
53	.034	.034	.218	.218	.126	.126	1.00	1.00	11.00	.00
54	.032	.032	.198	.198	.115	.115	1.00	1.00	12.00	.00
55	.029	.029	.180	.180	.104	.104	1.00	1.00	13.00	.00
56	.026	.026	.164	.164	.095	.095	1.00	1.00	14.00	.00
57	.024	.024	.149	.149	.086	.086	1.00	1.00	15.00	.00
58	.022	.022	.135	.135	.078	.078	1.00	1.00	16.00	.00
59	.020	.020	.122	.122	.071	.071	1.00	1.00	17.00	.00
60	.018	.018	.111	.111	.065	.065	1.00	1.00	18.00	.00
61	.016	.016	.101	.101	.059	.059	1.00	1.00	19.00	.00
62	.015	.015	.091	.091	.053	.053	1.00	1.00	20.00	.00
63	.013	.013	.083	.083	.048	.048	1.00	1.00	21.00	.00
64	.012	.012	.075	.075	.044	.044	1.00	1.00	22.00	.00
65	.011	.011	.068	.068	.040	.040	1.00	1.00	23.00	.00
66	.010	.010	.062	.062	.036	.036	1.00	1.00	24.00	.00
67	.009	.009	.056	.056	.032	.032	1.00	1.00	25.00	.00
68	.008	.008	.051	.051	.029	.029	1.00	1.00	26.00	.00
69	.007	.007	.046	.046	.027	.027	1.00	1.00	27.00	.00
70	.007	.007	.042	.042	.024	.024	1.00	1.00	28.00	.00
71	.006	.006	.038	.038	.022	.022	1.00	1.00	29.00	.00
72	.006	.006	.034	.034	.020	.020	1.00	1.00	30.00	.00
73	.005	.005	.031	.031	.018	.018	1.00	1.00	31.00	.00
74	.005	.005	.028	.028	.016	.016	1.00	1.00	32.00	.00
75	.004	.004	.025	.025	.015	.015	1.00	1.00	33.00	.00
76	.004	.004	.023	.023	.013	.013	1.00	1.00	34.00	.00
77	.003	.003	.021	.021	.012	.012	1.00	1.00	35.00	.00

..

FIVE.OUT

```
*****
*          N3DADE
*
*      ANALYTICAL SOLUTIONS FOR NONEQUILIBRIUM SOLUTE TRANSPORT
*      IN 3-D SEMI-INFINITE POROUS MEDIA
*
*      VOLUME-AVERAGED CONCENTRATIONS
*      Fig. 12: Heaviside production
*****

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MODEL PARAMETERS

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NAME	VALUE
------	-------

dimensional

V	5.00
R	1.00
Dx	5.00
Dy	2.00
Dz	2.00

dimensionless

BETA	.50
OMEGA	5.00
MU1	.50
MU2	.00

CONSTANTS

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=====

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L = 20.00

Co = .25

PRODUCTION VALUE PROBLEM 30

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=====

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HEAVISIDE PRODUCTION PROFILE

i	lam1	lam2	xin	xend
1	.50	1.00	.00	10.00

HEAVISIDE DISTRIBUTION FOR CIRCULAR GEOMETRY

i	rin	rend
1	.00	2.50

INDEPENDENT VARIABLES

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VARIABLE	INCREMENT	MINIMUM	MAXIMUM
t	.000	20.000	20.000
x	.125	.000	20.000
y	.125	.000	10.000
z	.000	.000	.000

PREDICTED CONCENTRATIONS

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=====

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NO	EQUILIBRIUM		NONEQUILIBRIUM		TOTAL		t	x	y	z
	C	C/Co	C	C/Co	C _t	C _t /Co				
1	.017	.069	.061	.246	.039	.157	20.00	.00	.00	.00
2	.017	.069	.061	.246	.039	.157	20.00	.00	.13	.00
3	.017	.069	.061	.246	.039	.157	20.00	.00	.25	.00
4	.017	.068	.061	.246	.039	.157	20.00	.00	.38	.00
5	.017	.068	.061	.245	.039	.157	20.00	.00	.50	.00

6	.017	.068	.061	.245	.039	.157	20.00	.00	.63	.00
7	.017	.067	.061	.245	.039	.156	20.00	.00	.75	.00
8	.017	.067	.061	.245	.039	.156	20.00	.00	.88	.00
9	.017	.067	.061	.244	.039	.155	20.00	.00	1.00	.00
10	.016	.066	.061	.244	.039	.155	20.00	.00	1.13	.00
11	.016	.065	.061	.243	.039	.154	20.00	.00	1.25	.00
12	.016	.064	.061	.243	.038	.153	20.00	.00	1.38	.00
13	.016	.063	.060	.242	.038	.152	20.00	.00	1.50	.00
14	.015	.061	.060	.241	.038	.151	20.00	.00	1.63	.00
15	.015	.059	.060	.239	.037	.149	20.00	.00	1.75	.00
16	.014	.056	.059	.237	.037	.147	20.00	.00	1.88	.00
17	.013	.053	.059	.235	.036	.144	20.00	.00	2.00	.00
18	.012	.048	.058	.232	.035	.140	20.00	.00	2.13	.00
19	.011	.043	.057	.229	.034	.136	20.00	.00	2.25	.00
20	.010	.038	.056	.225	.033	.132	20.00	.00	2.38	.00
21	.008	.033	.055	.222	.032	.127	20.00	.00	2.50	.00
22	.007	.027	.005	.018	.006	.023	20.00	.00	2.63	.00
23	.006	.022	.004	.015	.005	.019	20.00	.00	2.75	.00
24	.005	.018	.003	.012	.004	.015	20.00	.00	2.88	.00
25	.004	.015	.002	.010	.003	.012	20.00	.00	3.00	.00
26	.003	.012	.002	.008	.002	.010	20.00	.00	3.13	.00
27	.002	.009	.002	.006	.002	.008	20.00	.00	3.25	.00
28	.002	.008	.001	.005	.002	.006	20.00	.00	3.38	.00
29	.002	.006	.001	.004	.001	.005	20.00	.00	3.50	.00
30	.001	.005	.001	.004	.001	.005	20.00	.00	3.63	.00
31	.001	.005	.001	.003	.001	.004	20.00	.00	3.75	.00
32	.001	.004	.001	.003	.001	.003	20.00	.00	3.88	.00
33	.001	.004	.001	.002	.001	.003	20.00	.00	4.00	.00
34	.001	.003	.001	.002	.001	.003	20.00	.00	4.13	.00
35	.001	.003	.000	.002	.001	.002	20.00	.00	4.25	.00
36	.001	.002	.000	.002	.001	.002	20.00	.00	4.38	.00
37	.001	.002	.000	.001	.000	.002	20.00	.00	4.50	.00
38	.000	.002	.000	.001	.000	.002	20.00	.00	4.63	.00
39	.000	.002	.000	.001	.000	.001	20.00	.00	4.75	.00
40	.000	.001	.000	.001	.000	.001	20.00	.00	4.88	.00
41	.000	.001	.000	.001	.000	.001	20.00	.00	5.00	.00
42	.000	.001	.000	.001	.000	.001	20.00	.00	5.13	.00
43	.000	.001	.000	.001	.000	.001	20.00	.00	5.25	.00
44	.000	.001	.000	.001	.000	.001	20.00	.00	5.38	.00
45	.000	.001	.000	.000	.000	.001	20.00	.00	5.50	.00
46	.000	.001	.000	.000	.000	.000	20.00	.00	5.63	.00
47	.000	.000	.000	.000	.000	.000	20.00	.00	5.75	.00
48	.000	.000	.000	.000	.000	.000	20.00	.00	5.88	.00
49	.000	.000	.000	.000	.000	.000	20.00	.00	6.00	.00
50	.000	.000	.000	.000	.000	.000	20.00	.00	6.13	.00
51	.000	.000	.000	.000	.000	.000	20.00	.00	6.25	.00
52	.000	.000	.000	.000	.000	.000	20.00	.00	6.38	.00
53	.000	.000	.000	.000	.000	.000	20.00	.00	6.50	.00
54	.000	.000	.000	.000	.000	.000	20.00	.00	6.63	.00
55	.000	.000	.000	.000	.000	.000	20.00	.00	6.75	.00
56	.000	.000	.000	.000	.000	.000	20.00	.00	6.88	.00
57	.000	.000	.000	.000	.000	.000	20.00	.00	7.00	.00
58	.000	.000	.000	.000	.000	.000	20.00	.00	7.13	.00
59	.000	.000	.000	.000	.000	.000	20.00	.00	7.25	.00
60	.000	.000	.000	.000	.000	.000	20.00	.00	7.38	.00
61	.000	.000	.000	.000	.000	.000	20.00	.00	7.50	.00
62	.000	.000	.000	.000	.000	.000	20.00	.00	7.63	.00
63	.000	.000	.000	.000	.000	.000	20.00	.00	7.75	.00
64	.000	.000	.000	.000	.000	.000	20.00	.00	7.88	.00
65	.000	.000	.000	.000	.000	.000	20.00	.00	8.00	.00
66	.000	.000	.000	.000	.000	.000	20.00	.00	8.13	.00
67	.000	.000	.000	.000	.000	.000	20.00	.00	8.25	.00
68	.000	.000	.000	.000	.000	.000	20.00	.00	8.38	.00
69	.000	.000	.000	.000	.000	.000	20.00	.00	8.50	.00
70	.000	.000	.000	.000	.000	.000	20.00	.00	8.63	.00
71	.000	.000	.000	.000	.000	.000	20.00	.00	8.75	.00
72	.000	.000	.000	.000	.000	.000	20.00	.00	8.88	.00
73	.000	.000	.000	.000	.000	.000	20.00	.00	9.00	.00

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APPENDIX E. PROGRAM LISTING

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C ****
C *
C *          N3DADE
C *
C *      ANALYTICAL SOLUTIONS FOR NONEQUILIBRIUM SOLUTE
C *      TRANSPORT IN 3-D SEMI-INFINITE POROUS MEDIA
C *      JOURNAL OF HYDROLOGY 151:193-228
C *
C *      FEIKE J. LEIJ and NOBUO TORIDE
C *
C *      U.S. SALINITY LABORATORY
C *      450 W. BIG SPRINGS ROAD
C *      RIVERSIDE, CA 92507-4617
C *
C *      PHONE (909) 369-4851
C *      FAX   (909) 342-4964
C *
C *      MODIFIED: 4/97
C ****

IMPLICIT REAL*8(A-H,O-Z)
PARAMETER (ZIP=1.0D-10,ZERO=0.0D+00,ONE=1.0D+00)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,np,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/BVP/ NBP,T0B,DMB,GPB(10),TPB(10),GEB,ALB,JB
COMMON/IVP/ NIP,X01,DMI,FPI(10),XPI(10),FEI,ALI,JI
COMMON/PVP/ NPP,OLAM(10),TLAM(10),XPP(10),XOP,OLAME,TLAME,ALP,JP
COMMON/TRANS/ Y0,Z0,NYP,YP(5),NZP,ZP(5),ALY,ALZ
DIMENSION GP(5),TP(5),FP(5),XP(5),XD(4),XLOW(4),XUP(4),NXST(4),DX(
84)
CHARACTER TITLE*60,VN(4)*5,FILENAME*15
DATA VN/'t','x','y','z'/

C --- OPEN I/O FILES ---
WRITE(*, 150)
READ(*, 160) FILENAME
IF (FILENAME.EQ.' ') FILENAME='N3DADE.IN'
OPEN(5, FILE=FILENAME, STATUS='OLD')

C
WRITE(*,170)
READ(*,160) FILENAME
IF (FILENAME.EQ.' ') FILENAME='N3DADE.OUT'
OPEN(7, FILE=FILENAME, STATUS='UNKNOWN')

C --- CLEAR SCREEN AND WRITE TITLE ---
WRITE(*,190) FILENAME
READ(5,200) NC,NGC

C DO 120 NCASE=1,NC
C
READ(5,201) TITLE
READ(5,202) V,R,DCX,DCY,DCZ
READ(5,202) BETA,OMEGA,U1,U2
C
READ(5,204) UL,CO,MP,MC
IF(MC.EQ.1) THEN
  WRITE(7,300) TITLE
ELSE
  WRITE(7,299) TITLE
ENDIF
WRITE(7,210) V,R,DCX,DCY,DCZ,BETA,OMEGA,U1,U2
PX=V*UL/DCX
PY=V*UL/DCY
PZ=V*UL/DCZ
WRITE(7,301) UL,CO
OMU1=(OMEGA+U1)/BETA/R
OMU2=(OMEGA+U2)/(ONE-BETA)/R

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OM1=OMEGA/(ONE-BETA)/R
OM2=OMEGA/BETA/R
OMOM=OM1*OM2
U1R=U1/BETA/R
U2R=OMEGA*U2/(OMEGA+U2)/BETA/R
IF(MP.EQ.2) GOTO 3
IF(MP.EQ.3) GOTO 11
C
C --- BOUNDARY VALUE PROBLEM ---
READ(5,201) TITLE
READ(5,200) NP,NBP,NYP,NZP
WRITE(7,211) NP
C --- DIRAC ---
IF(NP.GE.1 .AND. NP.LE.9 .OR. NP.EQ.28 .OR. NP.EQ.29) THEN
  READ(5,202) TO,DBM
  WRITE(7,212) TO,DBM
  DMB=DBM/CO
  TOB=V*TO/UL
C --- HEAVISIDE ---
ELSE IF(NP.GE.10.AND.NP.LE.18.OR.NP.EQ.30.OR.NP.EQ.31)THEN
  WRITE(7,213)
  TP(1)=0.
  TPB(1)=0.
  READ(5,202) (GP(I),TP(I+1),I=1,NBP)
  DO 2 I=1,NBP
    WRITE(7,214) I,GP(I),TP(I),TP(I+1)
    GPB(I)=GP(I)/CO
2   TPB(I+1)=V*TP(I+1)/UL
C --- EXPONENTIAL ---
ELSE IF(NP.GE.19.AND.NP.LE.27.OR.NP.EQ.32.OR.NP.EQ.33)THEN
  READ(5,202) GE,ALB
  WRITE(7,215) GE,ALB
  GEB=GE/CO
ENDIF
GOTO 13
C
C --- INITIAL VALUE PROBLEM ---
3 READ(5,201) TITLE
READ(5,200) NP,NIP,NYP,NZP
WRITE(7,221) NP
C --- DIRAC ---
IF(NP.GE.1 .AND. NP.LE.9 .OR. NP.EQ.28 .OR. NP.EQ.29) THEN
  READ(5,202) X0,DMI
  WRITE(7,222) X0,DMI
  DMI=DMI/CO
  X0I=X0/UL
C --- HEAVISIDE ---
ELSE IF(NP.GE.10.AND.NP.LE.18.OR.NP.EQ.30.OR.NP.EQ.31)THEN
  WRITE(7,223)
  READ(5,202) XP(1),(FP(I),XP(I+1),I=1,NIP)
  XPI(1)=XP(1)/UL
  DO 4 I=1,NIP
    WRITE(7,214) I,FP(I),XP(I),XP(I+1)
    FPI(I)=FP(I)/CO
4   XPI(I+1)=XP(I+1)/UL
C --- EXPONENTIAL ---
ELSE IF(NP.GE.19.AND.NP.LE.27.OR.NP.EQ.32.OR.NP.EQ.33)THEN
  READ(5,202) FE,ALI
  WRITE(7,224) FE,ALI
  FEI=FE/CO
C --- spherical HEAVISIDE ---
ELSE IF(NP.EQ.34)THEN
  READ(5,202) X0,(FP(I),XP(I),I=1,NIP)
  X0I=X0/UL
  I=1
  FPI(I)=FP(I)/CO
  XPI(I)=XP(I)/UL
  WRITE(7,225) X0
  WRITE(7,214) I,FP(I),DUM,XP(I)
  DO 5 I=2,NIP

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      WRITE(7,214) I,FP(I),XP(I-1),XP(I)
      FP(I)=FP(I)/CO
  5   XPI(I)=XP(I)/UL
C   --- spherical EXPONENTIAL ---
ELSE IF(NP.EQ.35)THEN
  READ(5,202) X0,FE,ALI,BINT
  WRITE(7,226) X0,FE,ALI
  X0I=X0/UL
  BINT=BINT/UL
  FEI=FE/CO
ENDIF
GOTO 13
C
C   --- PRODUCTION VALUE PROBLEM ---
11 READ(5,201) TITLE
  READ(5,200) NP,NPP,NYP,NZP
  WRITE(7,231) NP
C   --- HEAVISIDE ---
IF(NP.EQ.14.OR.NP.EQ.15.OR.NP.EQ.17.OR.NP.EQ.18.OR.NP.EQ.
&.30.OR.NP.EQ.31) THEN
  WRITE(7,232)
  READ(5,202) XP(1),(OLAM(I),TLAM(I),XP(I+1),I=1,NPP)
  XPP(1)=XP(1)/UL
  DO 6 I=1,NPP
    WRITE(7,214) I,OLAM(I),TLAM(I),XP(I),XP(I+1)
  6   XPP(I+1)=XP(I+1)/UL
C   --- EXPONENTIAL ---
ELSE IF(NP.EQ.23.OR.NP.EQ.24.OR.NP.EQ.26.OR.NP.EQ.27.OR.NP.EQ.32
&.OR.NP.EQ.33) THEN
  READ(5,202) OLAME,TLAME,ALP
  WRITE(7,233) OLAME,TLAME,ALP
C   --- spherical HEAVISIDE ---
ELSE IF(NP.EQ.34)THEN
  READ(5,202) X0,(OLAM(I),TLAM(I),XP(I),I=1,NPP)
  DUM=0.
  I=1
  XOP=X0/UL
  XPP(1)=XP(1)/UL
  WRITE(7,234) X0
  WRITE(7,214) I,OLAM(I),TLAM(I),DUM,XP(I)
  DO 7 I=2,NPP
  7   WRITE(7,214) I,OLAM(I),TLAM(I),XP(I-1),XP(I)
C   --- spherical EXPONENTIAL ---
ELSE IF(NP.EQ.35)THEN
  READ(5,202) X0,OLAME,TLAME,ALP,BINT
  WRITE(7,235) X0,OLAME,TLAME,ALP
  XOP=X0/UL
  BINT=BINT/UL
ENDIF
C
C   --- TRANSVERSAL CONDITIONS ---
C   --- DIRAC/DIRAC ---
13 IF(NP.EQ.1 .OR. NP.EQ.10 .OR. NP.EQ.19) THEN
  READ(5,202) Y0
  WRITE(7,241) Y0
  READ(5,202) Z0
  WRITE(7,242) Z0
  Y0=Y0/UL
  Z0=Z0/UL
C   --- DIRAC/HEAVISIDE ---
ELSE IF(NP.EQ.2 .OR. NP.EQ.11 .OR. NP.EQ.20) THEN
  READ(5,202) Y0
  READ(5,202) (ZP(I),ZP(I+1),I=1,2*NZP,2)
  WRITE(7,241) Y0
  WRITE(7,244)
  DO 14 I=1,2*NZP,2
  14   WRITE(7,214) (I+1)/2,ZP(I),ZP(I+1)
  DO 814 I=1,2*NZP
  814   ZP(I)=ZP(I)/UL
  Y0=Y0/UL

```

```

C   --- DIRAC/EXPONENTIAL ---
ELSE IF(NP.EQ.3 .OR. NP.EQ.12 .OR. NP.EQ.21) THEN
READ(5,202) Y0
READ(5,202) ALZ,Z0
WRITE(7,241) Y0
WRITE(7,246) ALZ,Z0
Y0=Y0/UL
Z0=Z0/UL
C   --- HEAVISIDE/DIRAC ---
ELSE IF(NP.EQ.4 .OR. NP.EQ.13 .OR. NP.EQ.22) THEN
READ(5,202) (YP(I),YP(I+1),I=1,2*NYP,2)
READ(5,202) Z0
WRITE(7,243)
DO 15 I=1,2*NYP,2
15  WRITE(7,214) (I+1)/2,YP(I),YP(I+1)
DO 815 I=1,2*NYP
815  YP(I)=YP(I)/UL
WRITE(7,242) Z0
Z0=Z0/UL
C   --- HEAVISIDE/HEAVISIDE ---
ELSE IF(NP.EQ.5 .OR. NP.EQ.14 .OR. NP.EQ.23) THEN
READ(5,202) (YP(I),YP(I+1),I=1,2*NYP,2)
READ(5,202) (ZP(I),ZP(I+1),I=1,2*NZP,2)
WRITE(7,243)
DO 16 I=1,2*NYP,2
16  WRITE(7,214) (I+1)/2,YP(I),YP(I+1)
DO 816 I=1,2*NYP
816  YP(I)=YP(I)/UL
WRITE(7,244)
DO 17 I=1,2*NZP,2
17  WRITE(7,214) (I+1)/2,ZP(I),ZP(I+1)
DO 817 I=1,2*NZP
817  ZP(I)=ZP(I)/UL
C   --- HEAVISIDE/EXPONENTIAL ---
ELSE IF(NP.EQ.6 .OR. NP.EQ.15 .OR. NP.EQ.24) THEN
READ(5,202) (YP(I),YP(I+1),I=1,2*NYP,2)
READ(5,202) ALZ,Z0
WRITE(7,243)
DO 18 I=1,2*NYP,2
18  WRITE(7,214) (I+1)/2,YP(I),YP(I+1)
DO 818 I=1,2*NYP
818  YP(I)=YP(I)/UL
WRITE(7,246) ALZ,Z0
Z0=Z0/UL
C   --- EXPONENTIAL/DIRAC ---
ELSE IF(NP.EQ.7 .OR. NP.EQ.16 .OR. NP.EQ.25) THEN
READ(5,202) ALY,Y0
READ(5,202) Z0
WRITE(7,245) ALY,Y0
WRITE(7,242) Z0
Y0=Y0/UL
Z0=Z0/UL
C   --- EXPONENTIAL/HEAVISIDE ---
ELSE IF(NP.EQ.8 .OR. NP.EQ.17 .OR. NP.EQ.26) THEN
READ(5,202) ALY,Y0
WRITE(7,245) ALY,Y0
READ(5,202) (ZP(I),ZP(I+1),I=1,2*NZP,2)
WRITE(7,244)
DO 19 I=1,2*NZP,2
19  WRITE(7,214) (I+1)/2,ZP(I),ZP(I+1)
DO 819 I=1,2*NZP
819  ZP(I)=ZP(I)/UL
Y0=Y0/UL
C   --- EXPONENTIAL/EXPONENTIAL ---
ELSE IF(NP.EQ.9 .OR. NP.EQ.18 .OR. NP.EQ.27) THEN
READ(5,202) ALY,Y0
WRITE(7,245) ALY,Y0
Y0=Y0/UL
READ(5,202) ALZ,Z0
WRITE(7,246) ALZ,Z0

```

```

      Z0=Z0/UL
C   --- circular HEAVISIDE ---
ELSE IF(NP.EQ.28.OR. NP.EQ.30 .OR. NP.EQ.32) THEN
  READ(5,202) (YP(I),YP(I+1),I=1,2*NYP,2)
  WRITE(7,247)
  DO 20 I=1,2*NYP,2
  20  WRITE(7,214) (I+1)/2,YP(I),YP(I+1)
  DO 820 I=1,2*NYP
  820  YP(I)=YP(I)/UL
C   --- circular EXPONENTIAL ---
ELSE IF(NP.EQ.29.OR. NP.EQ.31 .OR. NP.EQ.33) THEN
  READ(5,202) ALY,BINT
  BINT=BINT/UL
  WRITE(7,248) ALY
ENDIF
C   --- CALCULATE NODE SPACING ---
WRITE(7,338)
DO 21 I=1,4
  READ(5,202) DX(I),XLOW(I),XUP(I)
  21  WRITE(7,340) VN(I),DX(I),XLOW(I),XUP(I)
C   WRITE(7,342) CHAR(12)
C   DO 23 I=1,4
    IF (ABS(DX(I)).LE.ZIP) THEN
      NXST(I)=1
    ELSE
      NXST(I)=ZIP+(XUP(I)+DX(I)-XLOW(I))/DX(I)
    ENDIF
  23 CONTINUE
C   NUM=0
  DO 22 I=1,NXST(1)
    XD(1)=XLOW(1)+(I-1)*DX(1)
    X(1)=XD(1)*V/UL
  DO 22 J=1,NXST(2)
    XD(2)=XLOW(2)+(J-1)*DX(2)
    X(2)=XD(2)/UL
  DO 22 K=1,NXST(3)
    XD(3)=XLOW(3)+(K-1)*DX(3)
    X(3)=XD(3)/UL
  DO 22 L=1,NXST(4)
    XD(4)=XLOW(4)+(L-1)*DX(4)
    X(4)=XD(4)/UL
    NUM=NUM+1
    Y1=ZERO
    Y2=ZERO
    CALL MODELS(Y1,Y2)
    YT=BETA*R*Y1+(ONE-BETA)*R*Y2
    YD1=Y1*CO
    YD2=Y2*CO
    YDT=YT*CO
    WRITE(7,346) NUM,YD1,Y1,YD2,Y2,YDT,YT,(XD(JJ),JJ=1,4)
  22 CONTINUE
  120 CONTINUE
C   --- END OF PROBLEM ---
150 FORMAT(' Enter input file name (default = N3DADE.IN)')
160 FORMAT(A15)
170 FORMAT(' Enter output file name (default = N3DADE.OUT)')
190 FORMAT(/////////////////5X,67(1H*)/5X,1H*,65X,1H*/5X,1H*,29X,'N3DAD
$E',30X,1H*/5X,1H*,65X,1H*/5X,1H*,4X,'PLEASE WAIT - The concentrati
$ons are being calculated and',4X,1H*/5x,1H*,18X,'written to ',A15,
$21X,1H*/5X,1H*,65X,1H*/5X,67(1H*)//)
200 FORMAT(5I5)
201 FORMAT(A60)
202 FORMAT(8F10.2)
204 FORMAT(2F10.2,2I10)
210 FORMAT(//5X,'MODEL PARAMETERS'/5X,16(1H=)//5X,'NAME',12X,'VALUE'//)

```

```

$5X,'dimensional'/5X,'V',10X,F10.2/5X,'R',10X,F10.2/5X,'Dx',9X,F10.
&2/5X,'Dy',9X,F10.2/5X,'Dz',9X,F10.2//5X,'dimensionless'/5X,'BETA',
&7X,F10.2/5X,'OMEGA',6X,F10.2/5X,'MU1',$8X,F
$10.2/5X,'MU2',8X,F10.2)
211 FORMAT(//5X,'BOUNDARY VALUE PROBLEM ',i5/5X,22(1H=))
212 FORMAT(5X,'DIRAC INPUT FUNCTION'/7X,'t0=',F10.2,8X,'m=',F10.2)
213 FORMAT(5X,'HEAVISIDE INPUT FUNCTION'/9X,'i',9X,'g',7X,'tin',6X,
&'tend')
214 FORMAT(5X,i5,6(F10.2))
215 FORMAT(5X,'EXPONENTIAL INPUT FUNCTION'/7X,'ge=',F10.2,4X,'alpha='
&,F10.2)
221 FORMAT(//5X,'INITIAL VALUE PROBLEM ',i5/5X,21(1H=))
222 FORMAT(5X,'DIRAC INITIAL DISTRIBUTION'/7X,'x0=',F10.2,8X,'m=',F10
$.2)
223 FORMAT(5X,'HEAVISIDE INITIAL DISTRIBUTION'/9X,'i',9X,'f',7X,'xin'
&,6X,'xend')
224 FORMAT(5X,'EXPONENTIAL INITIAL DISTRIBUTION'/7X,'fe=',F10.2,4X,'a
&lpha;',F10.2)
225 FORMAT(5X,'HEAVISIDE INITIAL DISTRIBUTION FOR SPHERICAL GEOMETRY
&x0=',F10.2/9X,'i',9X,'f',7X,'rin',6X,'rend')
226 FORMAT(5X,'EXPONENTIAL INITIAL DISTRIBUTION FOR SPHERICAL GEOMETRY
&y x0=',F10.2/7X,'fe=',F10.2,4X,'alpha=',F10.2)
231 FORMAT(//5X,'PRODUCTION VALUE PROBLEM ',i5/5X,24(1H=))
232 FORMAT(5X,'HEAVISIDE PRODUCTION PROFILE'/9X,'i',6X,'lam1',6X,'la
&m2',7X,'xin',6X,'xend')
233 FORMAT(5X,'EXPONENTIAL PRODUCTION PROFILE'/4X,'lam1e=',F10.2,4X,
&'lam2e=',F10.2,4X,'alpha=',F10.2)
234 FORMAT(5X,'HEAVISIDE PRODUCTION PROFILE FOR SPHERICAL GEOMETRY
&x0=',F10.2/9X,'i',6X,'lam1',6X,'lam2',7X,'rin',6X,'rend')
235 FORMAT(5X,'EXPONENTIAL INITIAL DISTRIBUTION FOR SPHERICAL GEOMETRY
&y x0=',F10.2/4X,'lam1e=',F10.2,4X,'lam2e=',F10.2,4X,'alpha='
&F10.2)
241 FORMAT(5X,'DIRAC DISTRIBUTION FOR Y-DIRECTION'/7X,'y0=',F10.2)
242 FORMAT(5X,'DIRAC DISTRIBUTION FOR Z-DIRECTION'/7X,'z0=',F10.2)
243 FORMAT(5X,'HEAVISIDE DISTRIBUTION FOR Y-DIRECTION'/9X,'i',7X,'yin
&,6X,'yend')
244 FORMAT(5X,'HEAVISIDE DISTRIBUTION FOR Z-DIRECTION'/9X,'i',7X,'zin
&,6X,'zend')
245 FORMAT(5X,'EXPONENTIAL DISTRIBUTION FOR Y-DIRECTION'/4X,'alpha='
&F10.2,4X,'y0=',F10.2)
246 FORMAT(5X,'EXPONENTIAL DISTRIBUTION FOR Z-DIRECTION'/4X,'alpha='
&F10.2,4X,'z0=',F10.2)
247 FORMAT(5X,'HEAVISIDE DISTRIBUTION FOR CIRCULAR GEOMETRY'/9X,'i',7
&X,'rin',6X,'rend')
248 FORMAT(5X,'EXPONENTIAL DISTRIBUTION FOR CIRCULAR GEOMETRY'/4X,'al
&pha;',F10.2)
299 FORMAT(//5X,67(1H*)/5X,1H*,65X,1H*/5X,1H*,29X,'N3DADE',30X,1H*/5X,
$1H*,65X,1H*/5X,1H*,4X,'ANALYTICAL SOLUTIONS FOR NONEQUILIBRIUM SOL
$UTE TRANSPORT',5X,1H*/5X,1H*,16X,'IN 3-D SEMI-INFINITE POROUS MEDI
$A',16X,1H*/5X,1H*,65X,1H*/5X,1H*,5X,'VOLUME-AVERAGED CONCENTRATION
$S',30X,1H*/5X,1H*,5X,A60,1H*/5X,1H*,65X,1H*/5X,67(1H*)
300 FORMAT(//5X,67(1H*)/5X,1H*,65X,1H*/5X,1H*,29X,'N3DADE',30X,1H*/5X,
$1H*,65X,1H*/5X,1H*,4X,'ANALYTICAL SOLUTIONS FOR NONEQUILIBRIUM SOL
$UTE TRANSPORT',5X,1H*/5X,1H*,16X,'IN 3-D SEMI-INFINITE POROUS MEDI
$A',16X,1H*/5X,1H*,65X,1H*/5X,1H*,5X,'FLUX-AVERAGED CONCENTRATIONS'
$,32X,1H*/5X,1H*,5X,A60,1H*/5X,1H*,65X,1H*/5X,67(1H*))
301 FORMAT(//5X,'CONSTANTS'/5X,9(1H=)/5X,'L_ =',F8.2/5X,'Co =',F8.2)
338 FORMAT(//5X,'INDEPENDENT VARIABLES'/5X,21(1H=)/5X,'VARIABLE',3X,'I
$INCREMENT',8X,'MINIMUM',8X,'MAXIMUM')
340 FORMAT(5X,A5,3(5X,F10.3))
342 FORMAT(A1/'PREDICTED CONCENTRATIONS'/24(1H=)//6X,'EQUILIBRIUM',3X
$','NONEQUILIBRIUM',5X,'TOTAL'/1X,'NO',4X,'C',5X,'C/Co',5X,'C',5X,'C
$/Co',5X,'Ct',4X,'Ct/Co',5X,'t',7X,'x',7X,'y',7X,'z')
346 FORMAT(14,3(F8.5,F7.5),4F8.2)
C
CLOSE(5)
CLOSE(7)
C
STOP
END

```

```

C
C -----
C      SUBROUTINE MODELS(Y1,Y2)
C
C      PURPOSE: TO CALCULATE EQUILIBRIUM AND NONEQUILIBRIUM CONCENTRATION
C
C      IMPLICIT REAL*8 (A-H,O-Z)
C      COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,np,BINT
C      COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
C      COMMON/BVP/ NBP,TOB,DMB,GPB(10),TPB(10),GEB,ALB,JB
C      COMMON/IVP/ NIP,XOI,DMI,FPI(10),XPI(10),FEI,ALI,JI
C      COMMON/PVP/ NPP,OLAM(10),TLAM(10),XPP(10),XOP,OLAME,TLAME,ALP,JP
C      COMMON/TRANS/ Y0,Z0,NYP,YP(5),NZP,ZP(5),ALY,ALZ
C      PARAMETER(ZIP=1.0D-8,ZERO=0.0D+00,ONE=1.0D+00,TWO=2.0D+00,
C      $ FOUR=4.0D+00,EIGHT=8.0D+00)
C      EXTERNAL DI1B,DI2B,HE1B,HE2B,EX1B,EX2B,
C      $DI1I,DI2I,HE1I,HE2I,EX1I,EX2I,H1S1I,H1S2I,H2S1I,E1S1I,E1S2I,E2S1I,
C      $HE1P,HE2P,EX1P,EX2P,H1S1P,H2SP,E1S1P,E2SP
C      PI=FOUR*DATAN(ONE)
C
C      Y1=0.
C      Y2=0.
C      IF(MP.EQ.2) GOTO 3
C      IF(MP.EQ.3) GOTO 11
C
C      --- BOUNDARY VALUE PROBLEM ---
C      --- DIRAC ---
C      IF(NP.GE.1 .AND. NP.LE.9 .OR. NP.EQ.28 .OR. NP.EQ.29) THEN
C          TT=X(1)-TOB
C          IF(TT.LE.ZERO) GOTO 103
C          Y1=DEXP(-OM2*TT)*GAMY(TT)*GAMZ(TT)*GB(X(2),TT)
C          CALL CHEB10(DI1B,RES,ZERO,TT,NGC)
C          Y1=DMB*(Y1+RES)
C          CALL CHEB10(DI2B,RES,ZERO,TT,NGC)
C          Y2=DMB*OM1*RES
C
C      --- HEAVISIDE ---
C      ELSE IF(NP.GE.10.AND.NP.LE.18.OR.NP.EQ.30.OR.NP.EQ.31)THEN
C          IF(X(1).LE.TPB(1)) GOTO 103
C          DO 31 JB=1,NBP
C              IF(X(1).GT.TPB(JB)) THEN
C                  IF(X(1).LE.TPB(JB+1)) THEN
C                      TLOW=0.
C                      TUP=X(1)-TPB(JB)
C                  ELSE
C                      TLOW=X(1)-TPB(JB+1)
C                      TUP=X(1)-TPB(JB)
C                  ENDIF
C              ELSE
C                  GOTO 32
C              ENDIF
C              CALL CHEB10(HE1B,RES1,TLOW,TUP,NGC)
C              CALL CHEB10(HE2B,RES2,TLOW,TUP,NGC)
C              Y1=Y1+GPB(JB)*RES1
C              Y2=Y2+GPB(JB)*RES2
C 31 CONTINUE
C 32 Y2=OMEGA*Y2/(OMEGA+U2)
C
C      --- EXPONENTIAL ---
C      ELSE IF (NP.GE.19.AND.NP.LE.27.OR.NP.EQ.32.OR.NP.EQ.33)THEN
C          CALL CHEB10(EX1B,RES,ZERO,X(1),NGC)
C          Y1=GEB*RES
C          CALL CHEB10(EX2B,RES,ZERO,X(1),NGC)
C          Y2=OM1*GEB*RES
C      ENDIF
C      GOTO 103
C
C      --- INITIAL VALUE PROBLEM ---
C      --- DIRAC ---
C 3 IF(NP.GE.1 .AND. NP.LE.9 .OR. NP.EQ.28 .OR. NP.EQ.29) THEN

```

```

YI=DEXP(-OM2*X(1))*GAMY(X(1))*GAMZ(X(1))*G(X0I,X(1),X(2))
CALL CHEB10(D1I1,RES,ZERO,X(1),NGC)
Y1=DMI*(YI+RES)

C
CALL CHEB10(D12I,RES,ZERO,X(1),NGC)
Y2=DMI*OM1*RES

C
--- HEAVISIDE ---
ELSE IF(NP.GE.10.AND.NP.LE.18.OR.NP.EQ.30.OR.NP.EQ.31)THEN
DO 34 JI=1,NIP
  if(x(1).le.zip) then
    if(x(2).ge.xpi(ji) .and. x(2).lt.xpi(ji+1)) y1=fpi(ji)
  & *YTRANS(X(3))*ZTRANS(X(4))
  else
    Y1I=DEXP(-OM2*X(1))*(G1(X(2),X(1),XPI(JI))
  & -G1(X(2),X(1),XPI(JI+1)))*GAMY(X(1))*GAMZ(X(1))
    CALL CHEB10(HE1I,RES1,ZERO,X(1),NGC)
    Y1=Y1+FPI(JI)*(Y1I+RES1)
  endif
  Y2I=0.
  IF(X(2).GE.XPI(JI).AND.X(2).LT.XPI(JI+1)) Y2I=YTRANS(X(3))
  & *ZTRANS(X(4))*DEXP(-OMU2*X(1))
  CALL CHEB10(HE2I,RES2,ZERO,X(1),NGC)
  Y2=Y2+FPI(JI)*(Y2I+OM1*RES2)
34 CONTINUE

C
--- EXPONENTIAL ---
ELSE IF(NP.GE.19.AND.NP.LE.27.OR.NP.EQ.32.OR.NP.EQ.33)THEN
  if(x(1).le.zip) then
    y1=fei*exp(-ali*x(2))*YTRANS(X(3))*ZTRANS(X(4))
  else
    Y1=YTRANS(X(3))*ZTRANS(X(4))*DEXP(-OM2*X(1))*G2(X(2),X(1),ALI)
    CALL CHEB10(EX1I,RES1,ZERO,X(1),NGC)
    Y1=FEI*(Y1+RES1)
  endif
  Y2=YTRANS(X(3))*ZTRANS(X(4))*DEXP(-ALI*X(2)-OMU2*X(1))
  CALL CHEB10(EX2I,RES2,ZERO,X(1),NGC)
  Y2=FEI*(Y2+OM1*RES2)

C
--- spherical HEAVISIDE ---
ELSE IF(NP.EQ.34)THEN
  RS=SQRT((X(2)-X0I)**2+X(3)**2+X(4)**2)
  JI=1
  RI=XPI(JI)
  if(x(1).le.zip) then
    if(rs.lt.xpi(ji)) then
      y1=fpi(ji)
    else
      do 77 i=2,nip
        if(rs.lt.xpi(i) .and. rs.ge.xpi(i-1)) y1=fpi(i)
    77 continue
    endif
  else
    BOT=X0I-RI
    TOP=X0I+RI
    CALL CHEB11(H1S1I,RI,RES1,BOT,TOP,NGC)
    CALL CHEB11(H1S2I,RI,RES2,ZERO,X(1),NGC)
    Y1=FPI(JI)*(DEXP(-OM2*X(1))*RES1+RES2)
  endif
  Y2I=0
  IF(RS.LT.XPI(JI)) Y2I=DEXP(-OMU2*X(1))
  CALL CHEB11(H2S1I,RI,RES,ZERO,X(1),NGC)
  Y2=FPI(JI)*(Y2I+OM1*RES)
  DO 35 JI=2,NIP
    RI=XPI(JI)
    BOT=X0I-RI
    TOP=X0I+RI
    CALL CHEB11(H1S1I,RI,RES1,BOT,TOP,NGC)
    CALL CHEB11(H1S2I,RI,RES2,ZERO,X(1),NGC)
    Y1=Y1+FPI(JI)*(DEXP(-OM2*X(1))*RES1+RES2)

```

```

Y2I=0.
IF(RS.GE.XPI(JI-1) .AND. RS.LT.XPI(JI)) Y2I=DEXP(-OMU2*X(1))
CALL CHEB11(H2S1I,RI,RES,ZERO,X(1),NGC)
Y2=FPI(JI)*(Y2I+OM1*RES)
RI=XPI(JI-1)
BOT=X0I-RI
TOP=X0I+RI
CALL CHEB11(H1S1I,RI,RES1,BOT,TOP,NGC)
CALL CHEB11(H1S2I,RI,RES2,ZERO,X(1),NGC)
Y1=Y1-FPI(JI)*(DEXP(-OM2*X(1))*RES1+RES2)
CALL CHEB11(H2S1I,RI,RES,ZERO,X(1),NGC)
Y2=Y2-FPI(JI)*OM1*RES
35 CONTINUE
C
C --- spherical EXPONENTIAL ---
ELSE IF(NP.EQ.35) THEN
  if(x(1).lt.zip) then
    Y1=FEI*DEXP(-ALI*SQRT((X(2)-X0I)**2+X(3)**2+X(4)**2))
  else
    bot=zero
    top=x0i+bint
    CALL CHEB10(E1S1I,res1,bot,top,NGC)
  endif
  CALL CHEB10(E1S2I,RES2,zero,x(1),NGC)
  Y1=FEI*(res1+RES2)
  CALL CHEB10(E2S1I,RES,zero,top,NGC)
  Y2=FEI*(DEXP(-OMU2*X(1)-ALI*SQRT((X(2)-X0I)**2+X(3)**2+X(4)**2))
& +OM1*RES)
C
  ENDIF
  GOTO 103
C
C --- PRODUCTION VALUE PROBLEM ---
C --- HEAVISIDE ---
11 IF(X(1).LT.ZIP) GOTO 103
IF(NP.EQ.14.OR.NP.EQ.15.OR.NP.EQ.17.OR.NP.EQ.18.OR.NP.EQ.30
& .OR.NP.EQ.31) THEN
  DO 36 JP=1,NPP
    CALL CHEB10(HE1P,RES,ZERO,X(1),NGC)
    Y1=Y1+RES
    Y2P=0.
    IF(X(2).GE.XPP(JP).AND.X(2).LT.XPP(JP+1)) Y2P=YTRANS(X(3))
    & *ZTRANS(X(4))*TLAM(JP)*(1-DEXP(-OMU2*X(1)))
    CALL CHEB10(HE2P,RES,ZERO,X(1),NGC)
    Y2=Y2P+OM2*RES
  36 CONTINUE
C
  Y1=Y1/BETA/R
  Y2=Y2/(OMEGA+U2)
C
C --- EXPONENTIAL ---
ELSE IF(NP.EQ.23.OR.NP.EQ.24.OR.NP.EQ.26.OR.NP.EQ.27.OR.NP.EQ.32
& .OR.NP.EQ.33) THEN
  CALL CHEB10(EX1P,RES,ZERO,X(1),NGC)
  Y1=RES/BETA/R
  Y2=YTRANS(X(3))*ZTRANS(X(4))*TLAME*DEXP(-ALP*X(2))
  & *(1-DEXP(-OMU2*X(1)))
  CALL CHEB10(EX2P,RES,ZERO,X(1),NGC)
  Y2=(Y2+OM2*RES)/(OMEGA+U2)
C
C --- spherical HEAVISIDE ---
ELSE IF(NP.EQ.34)THEN
  RS=SQRT((X(2)-X0P)**2+X(3)**2+X(4)**2)
  JP=1
  RI=XPP(JP)
  CALL CHEB11(H1S1P,RI,RES,ZERO,X(1),NGC)
  Y1=RES/BETA/R
  IF(RS.LT.XPP(JP)) Y2P=TLAM(JP)*(1-DEXP(-OMU2*X(1)))
  CALL CHEB11(H2SP,RI,RES,ZERO,X(1),NGC)
  Y2=(Y2P+OM2*RES)/(OMEGA+U2)

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DO 37 JP=2,NPP
  RI=XPP(JP)
  CALL CHEB11(H1S1P,RI,RES,ZERO,X(1),NGC)
  Y1=Y1+RES/BETA/R
  Y2P=0.
  IF(RS.LT.XPP(JP).AND.RS.GE.XPP(JP-1))
&   Y2P=TLAM(JP)*(1-DEXP(-OMU2*X(1)))
  CALL CHEB11(H2SP,RI,RES,ZERO,X(1),NGC)
  Y2=Y2+(Y2P+OM2*RES)/(OMEGA+U2)
  RI=XPP(JP-1)
  CALL CHEB11(H1S1P,RI,RES,ZERO,X(1),NGC)
  Y1=Y1-RES/BETA/R
  CALL CHEB11(H2SP,RI,RES,ZERO,X(1),NGC)
  Y2=Y2-OM2*RES/(OMEGA+U2)
37 CONTINUE
C
C --- spherical EXPONENTIAL ---
C ELSE IF(NP.EQ.35) THEN
  CALL CHEB10(E1S1P,RES,ZERO,X(1),NGC)
  Y1=RES/BETA/R
  CALL CHEB10(E2SP,RES,ZERO,X(1),NGC)
  Y2=TLAME*DEXP(-ALP*SQRT((X(2)-X0P)**2+X(3)**2+X(4)**2))
& *(1-DEXP(-OMU2*X(1)))+OM2*RES/(OMEGA+U2)
C
C ENDIF
103 CONTINUE
C
C RETURN
C
C AUXILIARY FUNCTIONS FOR LONG. EQ. AND NONEQ. PROBLEMS
C -----
FUNCTION DI1B(TAU)
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/BVP/ NBP,T0B,DMB,GPB(10),TPB(10),GEB,ALB,JB
PARAMETER (ZIP=1.0D-10,TWO=2.0D+00)
C
TT=X(1)-T0B
DUM=TT-TAU
IF(DUM.LT.ZIP) DUM=ZIP
P=TWO*DSQRT(DABS(OMOM*DUM*TAU))
Q=-OM2*TAU-OMU2*DUM
DI1B=DSQRT(OMOM*TAU/DUM)*EXPBI1(P,Q)*GAMY(TAU)*GAMZ(TAU)
&*GB(X(2),TAU)
C
RETURN
END
C
C -----
FUNCTION DI2B(TAU)
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/BVP/ NBP,T0B,DMB,GPB(10),TPB(10),GEB,ALB,JB
PARAMETER (TWO=2.0D+00)
C
TT=X(1)-T0B
P=TWO*DSQRT(DABS(OMOM*(TT-TAU)*TAU))
Q=-OMU2*(TT-TAU)-OM2*TAU
DI2B=EXPBIO(P,Q)*GB(X(2),TAU)*GAMY(TAU)*GAMZ(TAU)
RETURN
END
C
C -----
FUNCTION HE1B(TAU)
C

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IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/BVP/ NBP,TOB,DMB,GPB(10),TPB(10),GEB,ALB,JB
C
P=OMEGA*OMEGA*TAU/(OMEGA+U2)/BETA/R
Q=OMU2*(X(1)-TAU)
HE1B=GOLD(P,Q)*DEXP(-U2R*TAU)*GAMY(TAU)*GAMZ(TAU)*GB(X(2),TAU)
C
RETURN
END
C
-----
FUNCTION HE2B(TAU)
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/BVP/ NBP,TOB,DMB,GPB(10),TPB(10),GEB,ALB,JB
PARAMETER (ONE=1.0D+00)
C
P=OMEGA*OMEGA*TAU/(OMEGA+U2)/BETA/R
Q=OMU2*(X(1)-TAU)
HE2B=(ONE-GOLD(Q,P))*DEXP(-U2R*TAU)*GAMY(TAU)*GAMZ(TAU)
&*GB(X(2),TAU)
C
RETURN
END
C
-----
FUNCTION EX1B(TAU)
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/BVP/ NBP,TOB,DMB,GPB(10),TPB(10),GEB,ALB,JB
PARAMETER (ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
C
TT=X(1)-TAU
U=ALB-OMU2
IF(ABS(U).LE.ZIP) U=ZIP
EX1B=DEXP(-ALB*TT-OM2*TAU)*(DEXP(-OMOM*TAU/U)
& -DEXP(U*TT)*PHI1(TAU))*GAMY(TAU)*GAMZ(TAU)*GB(X(2),TAU)
C
RETURN
END
C
-----
FUNCTION EX2B(TAU)
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/BVP/ NBP,TOB,DMB,GPB(10),TPB(10),GEB,ALB,JB
PARAMETER (ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
C
TT=X(1)-TAU
U=ALB-OMU2
IF(ABS(U).LE.ZIP) U=ZIP
EX2B=DEXP(-OM2*TAU-OMU2*TT)*(DEXP(-OMOM*TAU/U)/U
& *(1-DEXP(-U*TT))-PHI2(TAU))*GAMY(TAU)*GAMZ(TAU)*GB(X(2),TAU)
C
RETURN
END
C
-----
FUNCTION DI1I(TAU)
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT

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COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/IVP/ NIP,XOI,DMI,FPI(10),XPI(10),FEI,ALI,JI
PARAMETER (ZIP=1.0D-10,TWO=2.0D+00)

C
TT=X(1)-TAU
IF(TT.LE.ZIP) TT=ZIP
P=TWO*DSQRT(OMOM*TT*TAU)
Q=-OM2*TAU-OMU2*TT
DI1I=(OM2*EXPBI0(P,Q)+DSQRT(OMOM*TAU/TT)*EXPBI1(P,Q))
$      *GAMY(TAU)*GAMZ(TAU)*G(XOI,TAU,X(2))

C
RETURN
END

C
-----
FUNCTION DI2I(TAU)

C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/IVP/ NIP,XOI,DMI,FPI(10),XPI(10),FEI,ALI,JI
PARAMETER (ONE=1.0D+00,TWO=2.0D+00,ZIP=1.0D-10)

C
TT=X(1)-TAU
IF(TT.LE.ZIP) TT=ZIP
DUM=TAU
IF(TAU.LE.ZIP) DUM=ZIP
P=TWO*DSQRT(OMOM*TT*TAU)
Q=-OM2*TAU-OMU2*TT
DI2I=(EXPBI0(P,Q)+DSQRT(OM2*TT/OM1/DUM)*EXPBI1(P,Q))
$      *GAMY(TAU)*GAMZ(TAU)*G(XOI,TAU,X(2))

C
RETURN
END

C
-----
FUNCTION HE1I(TAU)

C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/IVP/ NIP,XOI,DMI,FPI(10),XPI(10),FEI,ALI,JI
PARAMETER (ZIP=1.0D-10,TWO=2.0D+00)

C
TT=X(1)-TAU
IF(TT.LE.ZIP) TT=ZIP
P=TWO*DSQRT(OMOM*TT*TAU)
Q=-OM2*TAU-OMU2*TT
HE1I=(OM2*EXPBI0(P,Q)+DSQRT(OMOM*TAU/TT)*EXPBI1(P,Q))
$*(G1(X(2),TAU,XPI(JI))-G1(X(2),TAU,XPI(JI+1)))*GAMY(TAU)*GAMZ(TAU)

C
RETURN
END

C
-----
FUNCTION HE2I(TAU)

C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/IVP/ NIP,XOI,DMI,FPI(10),XPI(10),FEI,ALI,JI
PARAMETER (ZIP=1.0D-10,TWO=2.0D+00)

C
TT=X(1)-TAU
IF(TT.LE.ZIP) TT=ZIP
DUM=TAU
IF(TAU.LE.ZIP) DUM=ZIP
P=TWO*DSQRT(OMOM*TT*TAU)
Q=-OM2*TAU-OMU2*TT
HE2I=(EXPBI0(P,Q)+DSQRT(OM2*TT/OM1/DUM)*EXPBI1(P,Q))

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$*(G1(X(2),TAU,XPI(JI))-G1(X(2),TAU,XPI(JI+1)))*GAMY(TAU)*GAMZ(TAU)
C
RETURN
END
C
-----
FUNCTION EX1I(TAU)
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/IVP/ NIP,X0I,DMI,FPI(10),XPI(10),FEI,ALI,JI
PARAMETER (ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
C
TT=X(1)-TAU
IF(TT.LE.ZIP) TT=ZIP
DUM=TAU
IF(TAU.LE.ZIP) DUM=ZIP
P=TWO*DSQRT(OMOM*TT*TAU)
Q=-OM2*TAU-OMU2*TT
EX1I=(OM2*EXPBI0(P,Q)+DSQRT(OMOM*DUM/TT)*EXPBI1(P,Q))
$      *GAMY(TAU)*GAMZ(TAU)*G2(X(2),TAU,ALI)
C
RETURN
END
C
-----
FUNCTION EX2I(TAU)
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/IVP/ NIP,X0I,DMI,FPI(10),XPI(10),FEI,ALI,JI
PARAMETER (ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
C
TT=X(1)-TAU
IF(TT.LE.ZIP) TT=ZIP
DUM=TAU
IF(TAU.LE.ZIP) DUM=ZIP
P=TWO*DSQRT(OMOM*TT*TAU)
Q=-OM2*TAU-OMU2*TT
EX2I=(EXPBI0(P,Q)+DSQRT(OM2*TT/OM1/DUM)*EXPBI1(P,Q))
$      *GAMY(TAU)*GAMZ(TAU)*G2(X(2),TAU,ALI)
RETURN
END
C
-----
FUNCTION H1S1I(XI,RI)
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/IVP/ NIP,X0I,DMI,FPI(10),XPI(10),FEI,ALI,JI
PARAMETER (ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
C
H1S1I=GAM6(XI,X(3),X(4),X(1),RI,X0I)*G(XI,X(1),X(2))
C
RETURN
END
C
-----
FUNCTION H1S2I(TAU,RI)
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/IVP/ NIP,X0I,DMI,FPI(10),XPI(10),FEI,ALI,JI
PARAMETER (ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
EXTERNAL H1S3I

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TT=X(1)-TAU
IF(TT.LE.ZIP) TT=ZIP
P=TWO*DSQRT(OMOM*TAU*TT)
Q=-OM2*TAU-OMU2*TT
BOT=X0I-RI
TOP=X0I+RI
CALL CHEB21(H1S3I,TAU,RI,RES,bot,top,NGC)
H1S2I=(OM2*EXPBI0(P,Q)+DSQRT(OMOM*TAU/TT)*EXPBI1(P,Q))*RES
C
RETURN
END
C
----
FUNCTION H1S3I(TAU,XI,RI)
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/IVP/ NIP,X0I,DMI,FPI(10),XPI(10),FEI,ALI,JI
PARAMETER (ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
C
H1S3I=GAM6(XI,X(3),X(4),TAU,RI,X0I)*G(XI,TAU,X(2))
C
RETURN
END
C
----
FUNCTION H2S1I(TAU,RI)
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/IVP/ NIP,X0I,DMI,FPI(10),XPI(10),FEI,ALI,JI
PARAMETER (ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
EXTERNAL H2S2I
C
BOT=X0I-RI
TOP=X0I+RI
CALL CHEB21(H2S2I,TAU,RI,RES,bot,Top,NGC)
H2S1I=RES
C
RETURN
END
C
----
FUNCTION H2S2I(TAU,XI,RI)
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/IVP/ NIP,X0I,DMI,FPI(10),XPI(10),FEI,ALI,JI
PARAMETER (ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
C
H2S2I=GAM6(XI,X(3),X(4),TAU,RI,X0I)*G(XI,TAU,X(2))
C
RETURN
END
C
----
FUNCTION E1S1I(XI)
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/IVP/ NIP,X0I,DMI,FPI(10),XPI(10),FEI,ALI,JI
PARAMETER (ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
C
E1S1I=dexp(-om2*x(1))
$      *GAM7(XI,X(3),X(4),X(1),ALI,X0I)*G(XI,X(1),X(2))
C

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```

      RETURN
      END
C
C -----
FUNCTION E1S2I(XI)
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
      COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
      COMMON/IVP/ NIP,XOI,DMI,FPI(10),XPI(10),FEI,ALI,JI
      PARAMETER (ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
      EXTERNAL E1S3I
C
      CALL CHEB20(E1S3I,XI,RES,ZERO,X(1),NGC)
      E1S2I=RES
C
      RETURN
      END
C
C -----
FUNCTION E1S3I(XI,TAU)
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
      COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
      COMMON/IVP/ NIP,XOI,DMI,FPI(10),XPI(10),FEI,ALI,JI
      PARAMETER (ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
C
      TT=X(1)-TAU
      P=TWO*DSQRT(OMOM*TAU*TT)
      Q=-OM2*TAU-OMU2*TT
      E1S3I=(OM2*EXPBI0(P,Q)+DSQRT(OMOM*TAU/TT)*EXPBI1(P,Q))
      &      *GAM7(XI,X(3),X(4),TAU,ALI,XOI)*G(XI,TAU,X(2))
C
      RETURN
      END
C
C -----
FUNCTION E2S2I(XI)
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
      COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
      COMMON/IVP/ NIP,XOI,DMI,FPI(10),XPI(10),FEI,ALI,JI
      PARAMETER (ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
      EXTERNAL E2S2I
C
      CALL CHEB20(E2S2I,XI,RES,ZERO,X(1),NGC)
      E2S2I=RES
C
      RETURN
      END
C
C -----
FUNCTION E2S2I(XI,TAU)
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
      COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
      COMMON/IVP/ NIP,XOI,DMI,FPI(10),XPI(10),FEI,ALI,JI
      PARAMETER (ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
C
      IF(TT.LE.ZIP) TT=ZIP
      DUM=TAU
      TT=X(1)-TAU
      P=TWO*DSQRT(OMOM*TAU*TT)
      Q=-OM2*TAU-OMU2*TT
      E2S2I=(EXPBI0(P,Q)+DSQRT(OM2*TT/OM1/DUM)*EXPBI1(P,Q))
      &      *GAM7(XI,X(3),X(4),TAU,ALI,XOI)*G(XI,TAU,X(2))
C

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```

      RETURN
      END
C
C -----
FUNCTION HE1P(TAU)
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
      COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
      COMMON/PVP/ NPP,OLAM(10),TLAM(10),XPP(10),XOP,OLAME,TLAME,ALP,JP
      PARAMETER (ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
C
      DUM=TAU
      IF(TAU.LE.ZIP) DUM=ZIP
      TT=X(1)-TAU
      P=OMEGA*OMEGA*TAU/(OMEGA+U2)/BETA/R
      Q=OMU2*TT
C
      HE1P=DEXP(-U2R*TAU)*(OLAM(JP)*GOLD(P,Q)
      & +OMEGA*TLAM(JP)*(ONE-GOLD(Q,P))/(OMEGA+U2))
      & *(G1(X(2),TAU,XPP(JP))-G1(X(2),TAU,XPP(JP+1)))
      & *GAMY(TAU)*GAMZ(TAU)
C
      RETURN
      END
C
C -----
FUNCTION HE2P(TAU)
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
      COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
      COMMON/PVP/ NPP,OLAM(10),TLAM(10),XPP(10),XOP,OLAME,TLAME,ALP,JP
      PARAMETER (ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
C
      TT=X(1)-TAU
      IF(TT.LE.ZIP) TT=ZIP
      P=OMEGA*OMEGA*TAU/(OMEGA+U2)/BETA/R
      Q=OMU2*TT
      ARG1=TWO*DSQRT(P*Q)
      ARG2=-P-Q
      HE2P=DEXP(-U2R*TAU)*(OLAM(JP)*(GOLD(Q,P)-EXPBI0(arg1,arg2))
      & +OMEGA*TLAM(JP)*(1.-GOLD(Q,P)+SQRT(Q/P)*EXPBI1(ARG1,arg2))
      & /(OMEGA+U2))
      & *(G1(X(2),TAU,XPP(JP))-G1(X(2),TAU,XPP(JP+1)))
      & *GAMY(TAU)*GAMZ(TAU)
C
      RETURN
      END
C
C -----
FUNCTION EX1P(TAU)
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
      COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
      COMMON/PVP/ NPP,OLAM(10),TLAM(10),XPP(10),XOP,OLAME,TLAME,ALP,JP
      PARAMETER (ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
C
      TT=X(1)-TAU
      IF(TT.LE.ZIP) TT=ZIP
      P=OMEGA*OMEGA*TAU/(OMEGA+U2)/BETA/R
      Q=OMU2*TT
      EX1P=DEXP(-U2R*TAU)*(OLAME*GOLD(P,Q)
      & +OMEGA*TLAME*(ONE-GOLD(Q,P))/(OMEGA+U2))
      & *G2(X(2),TAU,ALP)*GAMY(TAU)*GAMZ(TAU)
C
      RETURN
      END

```

```

C ----
C FUNCTION EX2P(TAU)
C
C IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/PVP/ NPP,OLAM(10),TLAM(10),XPP(10),XOP,OLAME,TLAME,ALP,JP
PARAMETER (ZIP=1.0D-10,ZERO=0.0D+00,ONE=1.0D+00,TWO=2.0D+00)
C
C TT=X(1)-TAU
IF(TT.LE.ZIP) TT=ZIP
P=OMEGA*OMEGA*TAU/(OMEGA+U2)/BETA/R
Q=OMU2*TT
ARG1=TWO*DSQRT(P*Q)
ARG2=-P-Q
EX2P=DEXP(-U2R*TAU)*(OLAME*(GOLD(Q,P)-EXPBI0(arg1,arg2))
& +OMEGA*TLAME*(1.-GOLD(Q,P)+SQRT(Q/P)*EXPBI1(ARG1,arg2))
& /(OMEGA+U2))*G2(X(2),TAU,ALP)*GAMY(TAU)*GAMZ(TAU)
C
C RETURN
END
C ----
C FUNCTION H1S1P(TAU,RI)
C
C IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/PVP/ NPP,OLAM(10),TLAM(10),XPP(10),XOP,OLAME,TLAME,ALP,JP
PARAMETER (ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
EXTERNAL H1S2P
C
C TT=X(1)-TAU
IF(TT.LE.ZIP) TT=ZIP
P=OMEGA*OMEGA*TAU/(OMEGA+U2)/BETA/R
Q=OMU2*TT
C
BOT=XOP-RI
TOP=XOP+RI
CALL CHEB21(H1S2P,TAU,RI,RES,BOT,TOP,NGC)
C
H1S1P=DEXP(-U2R*TAU)*(OLAM(JP)*GOLD(P,Q)
& +OMEGA*TLAM(JP)*(ONE-GOLD(Q,P))/(OMEGA+U2))*RES
C
C RETURN
END
C ----
C FUNCTION H1S2P(TAU,XI,RI)
C
C IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/PVP/ NPP,OLAM(10),TLAM(10),XPP(10),XOP,OLAME,TLAME,ALP,JP
PARAMETER (ZERO=0.0D+00,ONE=1.0D+00,TWO=2.0D+00)
C
H1S2P=GAM6(XI,X(3),X(4),TAU,RI,XOP)*G(XI,TAU,X(2))
C
C RETURN
END
C ----
C FUNCTION H2SP(TAU,RI)
C
C IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/PVP/ NPP,OLAM(10),TLAM(10),XPP(10),XOP,OLAME,TLAME,ALP,JP
PARAMETER (ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
EXTERNAL H1S2P

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```

C
BOT=XOP-RI
TOP=XOP+RI
CALL CHEB21(H1S2P,TAU,RI,RES,BOT,TOP,NGC)
TT=X(1)-TAU
IF(TT.LE.ZIP) TT=ZIP
P=OMEGA*OMEGA*TAU/(OMEGA+U2)/BETA/R
Q=OMU2*TT
ARG1=TWO*DSQRT(P*Q)
ARG2=-P-Q
H2SP=RES*DEXP(-U2R*TAU)*(OLAM(JP)*(GOLD(Q,P)-EXPBI0(arg1,arg2))
& +OMEGA*TLAM(JP)*(1.-GOLD(Q,P)+SQRT(Q/P)*EXPBI1(ARG1,arg2))
& /(OMEGA+U2))

C
RETURN
END

C
C -----
FUNCTION E1S1P(TAU)

C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/PVP/ NPP,OLAM(10),TLAM(10),XPP(10),XOP,OLAME,TLAME,ALP,JP
PARAMETER (ZERO=0.0D+00,ONE=1.0D+00)
EXTERNAL E1S2P

C
BOT=ZERO
TOP=BINT
CALL CHEB20(E1S2P,TAU,RES,BOT,TOP,NGC)
TT=X(1)-TAU
P=OMEGA*OMEGA*TAU/(OMEGA+U2)/BETA/R
Q=OMU2*TT
E1S1P=DEXP(-U2R*TAU)*RES*(OLAME*GOLD(P,Q)
& +OMEGA*TLAME*(ONE-GOLD(Q,P))/(OMEGA+U2))

C
RETURN
END

C
C -----
FUNCTION E1S2P(TAU,XI)

C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/PVP/ NPP,OLAM(10),TLAM(10),XPP(10),XOP,OLAME,TLAME,ALP,JP
PARAMETER (ZERO=0.0D+00,ONE=1.0D+00)
E1S2P=GAM7(XI,X(3),X(4),TAU,ALP,XOP)*G(XI,TAU,X(2))

C
RETURN
END

C
C -----
FUNCTION E2SP(TAU)

C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/PVP/ NPP,OLAM(10),TLAM(10),XPP(10),XOP,OLAME,TLAME,ALP,JP
PARAMETER (ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00)
EXTERNAL E1S1P

C
BOT=ZERO
TOP=BINT
CALL CHEB20(E1S1P,TAU,RES,BOT,TOP,NGC)
TT=X(1)-TAU
IF(TT.LE.ZIP) TT=ZIP
P=OMEGA*OMEGA*TAU/(OMEGA+U2)/BETA/R
Q=OMU2*TT

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```

ARG1=TWO*DSQRT(P*Q)
ARG2=-P-Q
E2SP=DEXP(-U2R*TAU)*RES*(OLAME*(GOLD(Q,P)-EXPBI0(arg1,arg2))
& +OMEGA*TLAME*(1.-GOLD(Q,P)+SQRT(Q/P)*EXPBI1(ARG1,arg2))
& /(OMEGA+U2))
C
RETURN
END
C
C LONGITUDINAL AUXILIARY EXPRESSIONS (Table 2)
C -----
REAL*8 FUNCTION GB(XX,T)
C
IMPLICIT REAL*8 (A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
PARAMETER(ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
PI=FOUR*Datan(ONE)
C
DUM=T
IF(DUM.LT.ZIP) DUM=ZIP
IF (MC.EQ.1) THEN
  GB=XX*DSQRT(BETA*R*PX/FOUR/PI/DUM/DUM/DUM)
$ *DEXP(-U1R*T-PX*(BETA*R*XX-T)**2/FOUR/BETA/R/DUM)
ELSE
  GB=DEXP(-U1R*T)*(DSQRT(PX/PI/BETA/R/DUM)
$ *DEXP(-PX*(BETA*R*XX-T)**2/FOUR/BETA/R/DUM)
$ -PX/TWO/BETA/R*DEXP(PX*XX)*ERFC((BETA*R*XX+T)/
$ DSQRT(FOUR*BETA*R*DUM/PX)))
ENDIF
C
RETURN
END
C
C -----
REAL*8 FUNCTION G(XI,T,XX)
C
IMPLICIT REAL*8 (A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
PARAMETER(ZIP=1.0D-10,HALF=0.5D+00,ONE=1.0D+00,TWO=2.0D+00,
$FOUR=4.0D+00)
PI=FOUR*Datan(ONE)
C
DUM=T
IF(DUM.LT.ZIP) DUM=ZIP
C
IF (MC.EQ.1) THEN
  G=DEXP(-U1R*T)
$ *DSQRT(BETA*R*PX/FOUR/PI/DUM)*((ONE-(BETA*R*(XI-XX)+T)/
$ (TWO*DUM))*DEXP(-PX*(BETA*R*(XI-XX)+T)**2/FOUR/BETA/R/DUM)
$ -(ONE-(BETA*R*(XI+XX)+T)/TWO/DUM)*DEXP(PX*XX-PX*(BETA*R
$ *(XI+XX)+T)**2/FOUR/BETA/R/DUM))
ELSE
  G=(DSQRT(BETA*R*PX/FOUR/PI/DUM)*DEXP(PX*XX-PX*(BETA*R*(XI+
$ XX)+T)**2/FOUR/BETA/R/DUM)-HALF*PX*DEXP(PX*XX)*ERFC((BETA*
$ R*(XI+XX)+T)/DSQRT(FOUR*BETA*R*DUM/PX))+DSQRT(BETA*R*PX/
$ FOUR/PI/DUM)*DEXP(-PX*(BETA*R*(XI-XX)+T)**2/FOUR/BETA/R/
$ DUM))*DEXP(-U1R*T)
ENDIF
C
RETURN
END
C
C -----
REAL*8 FUNCTION G1(XX,T,XXI)
C
IMPLICIT REAL*8 (A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R

```

```

PARAMETER(ZIP=1.0D-10, HALF=0.5D+00, ONE=1.0D+00, FOUR=4.0D+00)
PI=FOUR*Datan(ONE)

C
DUM=T
IF(DUM.LT.ZIP) DUM=ZIP

C
IF (MC.EQ.1) THEN
  G1=DEXP(-U1R*T)*(ONE-HALF*ERFC((BETA*R*(XX-XXI)-T)/DSQRT(FOUR
$ *BETA*R*DUM/PX))-HALF*DEXP(PX*XX)*ERFC((BETA*R*(XX+XXI)+T)
$ /DSQRT(FOUR*BETA*R*DUM/PX))-DSQRT(BETA*R/FOUR/PI/DUM/PX)
$ *DEXP(-PX*(BETA*R*(XX-XXI)-T)**2/FOUR/BETA/R/DUM)
$ +DSQRT(BETA*R/FOUR/PI/DUM/PX)*DEXP(PX*XX)
$ *DEXP(-PX*(BETA*R*(XX+XXI)+T)**2/FOUR/BETA/R/DUM))
ELSE
  G1=(ONE-HALF*ERFC((BETA*R*(XX-XXI)-T)/DSQRT(FOUR*BETA*R*DUM/PX))
$ +HALF*(ONE+PX*(XX+XXI)+PX*T/BETA/R)*DEXP(PX*XX)*ERFC(
$ BETA*R*(XX+XXI)+T)/DSQRT(FOUR*BETA*R*DUM/PX))-DSQRT(PX*T/PI
$ /BETA/R)*DEXP(PX*XX-PX*(BETA*R*(XX+XXI)+T)**2/FOUR/BETA
$ /R/DUM))*DEXP(-U1R*T)
ENDIF

C
RETURN
END

C
-----
REAL*8 FUNCTION G2(XX,T,AL)
C
IMPLICIT REAL*8 (A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
PARAMETER(ZIP=1.0D-10, HALF=0.5D+00, ONE=1.0D+00, TWO=2.0D+00,
$ FOUR=4.0D+00)
PI=FOUR*Datan(ONE)

C
DUM=T
IF(DUM.LT.ZIP) DUM=ZIP

C
IF (MC.EQ.1) THEN
  G2=(ONE+AL/PX)*DEXP((AL+AL**2/PX-U1)*T/BETA/R)*
$ (DEXP(-AL*XX)*(ONE-HALF*ERFC((BETA*R*XX-T*(ONE+TWO*AL/
$ PX))/DSQRT(FOUR*BETA*R*DUM/PX)))+HALF*DEXP((AL+PX)*XX)*ERFC(
$ ((BETA*R*XX+T*(ONE+TWO*AL/PX))/DSQRT(FOUR*BETA*R*DUM/PX)))
ELSE
  G2=DEXP((AL+AL**2/PX-U1)*T/(BETA*R))*(DEXP(-AL*XX)*(ONE-
$ HALF*ERFC((BETA*R*XX-T*(ONE+TWO*AL/PX))/DSQRT(FOUR*BETA*R*
$ DUM/PX)))+HALF*(ONE+PX/AL)*DEXP((AL+PX)*XX)*ERFC((BETA*R*
$ XX+T*(ONE+TWO*AL/PX))/DSQRT(FOUR*BETA*R*DUM/PX)))-(HALF*PX/
$ AL)*EXP(PX*XX-U1*T/BETA/R)*ERFC((BETA*R*XX+T)/DSQRT(FOUR*BETA*R
$ *DUM/PX))
ENDIF

C
RETURN
END

C
TRANSVERSE AUXILIARY EXPRESSIONS (Table 3)
C
-----
REAL*8 FUNCTION GAMY(T)
C
IMPLICIT REAL*8 (A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/TRANS/ Y0,Z0,NYP,YP(5),Nzp,ZP(5),ALY,ALZ
PARAMETER (ZIP=1.0D-10, ONE=1.0D+00, FOUR=4.0D+00)
EXTERNAL GAM4,GAM5

C
PI=FOUR*Datan(ONE)

C
IF(T.LT.ZIP) T=ZIP

C
DIRAC

```

```

IF(NP.EQ.1.OR.NP.EQ.2.OR.NP.EQ.3.OR.NP.EQ.10.OR.NP.EQ.11.OR.
& NP.EQ.12.OR.NP.EQ.19.OR.NP.EQ.20.OR.NP.EQ.21) THEN
  GAMY=DSQRT(BETA*R*PY/FOUR/PI/T)*DEXP(-BETA*R*PY*(X(3)-Y0)**2
& /FOUR/T)

C
C HEAVISIDE
ELSE IF (NP.EQ.4.OR.NP.EQ.5.OR.NP.EQ.6.OR.NP.EQ.13.OR.NP.EQ.14.OR.
& NP.EQ.15.OR.NP.EQ.22.OR.NP.EQ.23.OR.NP.EQ.24) THEN
  SUMY=0.
DO 11 I=1,2*NYP,2
  SUMY=SUMY+0.5*ERFC(DSQRT(BETA*R*PY/FOUR/T)*(X(3)-YP(I+1)))
& -0.5*ERFC(DSQRT(BETA*R*PY/FOUR/T)*(X(3)-YP(I)))
11 CONTINUE
  GAMY=SUMY

C
C EXPONENTIAL
ELSE IF (NP.EQ.7.OR.NP.EQ.8.OR.NP.EQ.9.OR.NP.EQ.16.OR.NP.EQ.17.OR.
& NP.EQ.18.OR.NP.EQ.25.OR.NP.EQ.26.OR.NP.EQ.27) THEN
  GAMY=0.5*DEXP(ALY*(Y0-X(3))+ALY*ALY*T/BETA/R/PY)
& *ERFC((BETA*R*PY*(Y0-X(3))+2*ALY*T)/sqrt(4.*BETA*R*PY*T))
& +0.5*DEXP(ALY*(X(3)-Y0)+ALY*ALY*T/BETA/R/PY)
& *ERFC((BETA*R*PY*(X(3)-Y0)+2*ALY*T)/sqrt(4.*BETA*R*PY*T))

C
C circular HEAVISIDE
ELSE IF (NP.EQ.28.OR.NP.EQ.30.OR.NP.EQ.32) THEN
  SUMY=0.
DO 12 I=1,2*NYP,2
  IF(YP(I).LE.ZIP) THEN
    RES=0.
  ELSE
    BOT=X(3)-YP(I)
    TOP=X(3)+YP(I)
    CALL CHEB12(GAM4,T,YP(I),RES,BOT,TOP,NGC)
  ENDIF
  SUMY=RES+SUMY
  BOT=X(3)-YP(I+1)
  TOP=X(3)+YP(I+1)
  CALL CHEB12(GAM4,T,YP(I+1),RES,BOT,TOP,NGC)
  SUMY=RES-SUMY
12 CONTINUE
  GAMY=SUMY

C
C circular EXPONENTIAL
ELSE IF (NP.EQ.29.OR.NP.EQ.31.OR.NP.EQ.33) THEN
  BOT=-BINT
  TOP=BINT
  CALL CHEB11(GAM5,T,RES,BOT,TOP,NGC)
  GAMY=RES
  ENDIF

C
C RETURN
END

C -----
REAL*8 FUNCTION GAMZ(T)

C
IMPLICIT REAL*8 (A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/TRANS/ Y0,Z0,NYP,YP(5),NZP,ZP(5),ALY,ALZ
PARAMETER (ZIP=1.0D-10,ONE=1.0D+00,FOUR=4.0D+00)
PI=FOUR*DATAN(ONE)

C
IF(T.LT.ZIP) T=ZIP

C
DIRAC
IF(NP.EQ.1.OR.NP.EQ.10.OR.NP.EQ.19.OR.NP.EQ.4.OR.NP.EQ.13.OR.
& NP.EQ.22.OR.NP.EQ.7.OR.NP.EQ.16.OR.NP.EQ.25) THEN
  GAMZ=DSQRT(BETA*R*PZ/FOUR/PI/T)*DEXP(-BETA*R*PZ*(X(4)-Z0)**2
& /FOUR/T)

```

```

C
C      HEAVISIDE
C      ELSE IF(NP.EQ.2.OR.NP.EQ.11.OR.NP.EQ.20.OR.NP.EQ.5.OR.NP.EQ.14.OR.
&      NP.EQ.23.OR.NP.EQ.8.OR.NP.EQ.17.OR.NP.EQ.26) THEN
      SUMZ=0.
      DO 11 I=1,2*NZP,2
      SUMZ=SUMZ+0.5*ERFC(DSQRT(BETA*R*PZ/FOUR/T)*(X(4)-ZP(I+1)))
      &      -0.5*ERFC(DSQRT(BETA*R*PZ/FOUR/T)*(X(4)-ZP(I)))
11    CONTINUE
      GAMZ=SUMZ

C
C      EXPONENTIAL
C      ELSE IF(NP.EQ.3.OR.NP.EQ.12.OR.NP.EQ.21.OR.NP.EQ.6.OR.NP.EQ.15.OR.
&      NP.EQ.24.OR.NP.EQ.9.OR.NP.EQ.18.OR.NP.EQ.27) THEN
      GAMZ=0.5*DEXP(ALZ*(Z0-X(4))+ALZ*ALZ*T/BETA/R/PZ)
      &      *ERFC((BETA*R*PZ*(Z0-X(4))+2*ALZ*T)/sqrt(4.*BETA*R*PZ*T))
      &      +0.5*DEXP(ALZ*(X(4)-Z0)+ALZ*ALZ*T/BETA/R/PZ)
      &      *ERFC((BETA*R*PZ*(X(4)-Z0)+2*ALZ*T)/sqrt(4.*BETA*R*PZ*T))

C
C      circular
C      ELSE IF (NP.GE.28) THEN
      GAMZ=1.0
      ENDIF

C
C      RETURN
C      END

C
C      functions
C      -----
REAL*8 FUNCTION YTRANS(Y)

C
C      PURPOSE: DETERMINE DISTRIBUTION IN Y- OR RADIAL DIRECTION

C
C      IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/TRANS/ Y0,Z0,NYP,YP(5),NZP,ZP(5),ALY,ALZ
PARAMETER (ZERO=0.0D+00)

C
C      YTRANS=0.

C
C      HEAVISIDE
C      IF (NP.EQ.4.OR.NP.EQ.5.OR.NP.EQ.6.OR.NP.EQ.13.OR.NP.EQ.14.OR.
&NP.EQ.15.OR.NP.EQ.22.OR.NP.EQ.23.OR.NP.EQ.24
&.OR. NP.EQ.28 .OR. NP.EQ.30 .OR. NP.EQ.32) THEN
      DO 11 I=1,2*NYP,2
      IF(Y.GE.YP(I) .AND. Y.LE.YP(I+1)) YTRANS=1.

11    CONTINUE

C
C      EXPONENTIAL
C      ELSE IF (NP.EQ.7.OR.NP.EQ.8.OR.NP.EQ.9.OR.NP.EQ.16.OR.NP.EQ.17.OR.
&NP.EQ.18.OR.NP.EQ.25.OR.NP.EQ.26.OR.NP.EQ.27) THEN
      YTRANS=DEXP(-ALY*DABS(Y-Y0))

C
C      circular EXPONENTIAL
C      ELSE IF (NP.EQ.29 .OR. NP.EQ.31 .OR. NP.EQ.33) THEN
      YTRANS=DEXP(-ALY*Y)
      ENDIF

C
C      RETURN
C      END

C
C      -----
FUNCTION ZTRANS(Z)

C
C      PURPOSE: DETERMINE DISTRIBUTION IN Z-DIRECTION

C
C      IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R

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```

COMMON/TRANS/ Y0,Z0,NYP,YP(5),NZP,ZP(5),ALY,ALZ
PARAMETER (ZERO=0.0D+00)
C
C      ZTRANS=0.
C
C      HEAVISIDE
IF (NP.EQ.2.OR.NP.EQ.11.OR.NP.EQ.20.OR.NP.EQ.5.OR.NP.EQ.14.OR.
& NP.EQ.23.OR.NP.EQ.8.OR.NP.EQ.17.OR.NP.EQ.26) THEN
DO 11 I=1,2*NZP,2
  IF(Z.GE.ZP(I) .AND. Z.LE.ZP(I+1)) ZTRANS=1.
11  CONTINUE
C
C      circular HEAVISIDE
ELSE IF (NP.EQ.28 .OR. NP.EQ.30 .OR. NP.EQ.32) THEN
  ZTRANS=1.
C
C      EXPONENTIAL
ELSE IF (NP.EQ.3.OR.NP.EQ.12.OR.NP.EQ.21.OR.NP.EQ.6.OR.NP.EQ.15
& .OR.NP.EQ.24.OR.NP.EQ.9.OR.NP.EQ.18.OR.NP.EQ.27) THEN
  ZTRANS=DEXP(-ALZ*DABS(Z-Z0))
C
C      circular EXPONENTIAL
ELSE IF (NP.EQ.29 .OR. NP.EQ.31 .OR. NP.EQ.33) THEN
  ZTRANS=1.
ENDIF
C
C      RETURN
END
C
C -----
REAL*8 FUNCTION GAM4(PHI,T,RI)
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/TRANS/ Y0,Z0,NYP,YP(5),NZP,ZP(5),ALY,ALZ
PARAMETER(ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
PI=FOUR*DATAN(ONE)
C
IF(T.LT.ZIP) T=ZIP
C
GAM4=DSQRT(BETA*R*PY/PI/T)*DEXP(-BETA*R*PY*PHI*PHI/FOUR/T)
$    *(ERFC(DSQRT(BETA*R*PZ/FOUR/T)*(X(4)-DSQRT(DABS(RI*RI-(X(3)
$    -PHI)**2))))-ERFC(DSQRT(BETA*R*PZ/FOUR/T)*(X(4)+DSQRT(DABS
$    (RI*RI-(X(3)-PHI)**2)))))/FOUR
C
RETURN
END
C
C -----
REAL*8 FUNCTION GAM5(PHI,T)
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/TRANS/ Y0,Z0,NYP,YP(5),NZP,ZP(5),ALY,ALZ
PARAMETER(ONE=1.0D+00,FOUR=4.0D+00)
EXTERNAL GAM51
C
PI=FOUR*DATAN(ONE)
C
BOT=-BINT
TOP=BINT
C
CALL CHEB21(GAM51,PHI,T,RES,BOT,TOP,NGC)
GAM5=RES
C
RETURN
END
C

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```

C -----
C      REAL*8 FUNCTION GAM51(PHI,OME,T)
C
C      IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/TRANS/ Y0,Z0,NYP,YP(5),Nzp,ZP(5),ALY,ALZ
PARAMETER(ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
PI=FOUR*DATAN(ONE)
C
C      IF(T.LT.ZIP) T=ZIP
C
C      GAM51=(BETA*R*DSQRT(PY*PZ)/PI/T/FOUR)
& *DEXP(-ALY*DSQRT((X(3)-PHI)**2+(X(4)-OME)**2))
& -BETA*R*(PY*PHI*PHI+PZ*OME*OME)/FOUR/T)
C
C      RETURN
END
C -----
C      REAL*8 FUNCTION GAM6(XI,Y,Z,T,RI,X0)
C
C      IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/TRANS/ Y0,Z0,NYP,YP(5),Nzp,ZP(5),ALY,ALZ
PARAMETER(ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
EXTERNAL GAM61
PI=FOUR*DATAN(ONE)
C
C      IF(T.LE.ZIP) T=ZIP
BOT=X(3)-SQRT(RI*RI-(XI-X0)**2)
TOP=X(3)+SQRT(RI*RI-(XI-X0)**2)
C
CALL CHEB25(GAM61,XI,Y,Z,T,RI,X0,RES,BOT,TOP,NGC)
GAM6=RES
C
RETURN
END
C -----
C      REAL*8 FUNCTION GAM61(XI,PHI,Y,Z,T,RI,X0)
C
C      IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/TRANS/ Y0,Z0,NYP,YP(5),Nzp,ZP(5),ALY,ALZ
PARAMETER(ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
PI=FOUR*DATAN(ONE)
C
IF(T.LE.ZIP) T=ZIP
GAM61=DSQRT(BETA*R*PY/PI/T)*DEXP(-BETA*R*PY*PHI*PHI/FOUR/T)
$   *(ERFC(DSQRT(BETA*R*PZ/FOUR/T)*(Z-DSQRT(DABS(RI*RI
$   -(XI-X0)**2-(Y-PHI)**2)))))-ERFC(DSQRT(BETA*R*PZ/FOUR/T
$   *(Z+DSQRT(DABS(RI*RI-(XI-X0)**2-(Y-PHI)**2)))))/FOUR
C
RETURN
END
C -----
C      REAL*8 FUNCTION GAM7(XI,Y,Z,T,AL,X0)
C
C      IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/TRANS/ Y0,Z0,NYP,YP(5),Nzp,ZP(5),ALY,ALZ
PARAMETER(ZERO=0.0D+00,ONE=1.0D+00,FOUR=4.0D+00)
EXTERNAL GAM71
C
PI=FOUR*DATAN(ONE)

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```

C
C      GAM7=0.
C      BOT=-BINT
C      TOP=bint
C
C      CALL CHEB25(GAM71,XI,Y,Z,T,AL,X0,RES,BOT,TOP,NGC)
C      GAM7=RES+GAM7
C
C      RETURN
C      END
C
C      -----
C      REAL*8 FUNCTION GAM71(XI,PHI,Y,Z,T,AL,X0)
C
C      IMPLICIT REAL*8(A-H,O-Z)
C      COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
C      COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
C      COMMON/TRANS/ Y0,Z0,NYP,YP(5),Nzp,ZP(5),ALY,ALZ
C      PARAMETER(ZERO=0.0D+00,ONE=1.0D+00,FOUR=4.0D+00)
C      EXTERNAL GAM72
C
C      GAM71=0.
C      BOT=-BINT
C      TOP=bint
C
C      CALL CHEB35(GAM72,XI,PHI,Y,Z,T,AL,X0,RES,BOT,TOP,NGC)
C      GAM71=RES+GAM71
C
C      RETURN
C      END
C
C      -----
C      REAL*8 FUNCTION GAM72(XI,PHI,OME,Y,Z,T,AL,X0)
C
C      IMPLICIT REAL*8(A-H,O-Z)
C      COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
C      COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
C      COMMON/TRANS/ Y0,Z0,NYP,YP(5),Nzp,ZP(5),ALY,ALZ
C      PARAMETER(ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
C      PI=FOUR*DATAN(ONE)
C
C      if(t.lt.zip) t=zip
C      GAM72=(BETA*R*DSQRT(PY*PZ)/PI/t/FOUR)
C      & *DEXP(-AL*DSQRT((XI-X0)**2+(Y-PHI)**2+(Z-OME)**2)
C      & -BETA*R*(PY*PHI*PHI+PZ*OME*OME)/FOUR/t)
C
C      RETURN
C      END
C
C      -----
C      INTEGRATION ROUTINES
C
C      SUBROUTINE CHEB10(FUNC,AREA,A,B,M)
C
C      PURPOSE: PERFORM INTEGRATION OF F(X) BETWEEN A AND B
C              USING M-POINT GAUSS-CHEBYSHEV QUADRATURE FORMULA
C
C      IMPLICIT REAL*8 (A-H,O-Z)
C      PARAMETER(ZERO=0.0D+00,ONE=1.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
C      PI=FOUR*DATAN(ONE)
C      AREA=ZERO
C      SUM=ZERO
C      DO 10 I=1,M
C          Z1=DCOS(DFLOAT(2*(I-1)+1)*PI/DFLOAT(2*M))
C          VAR1=(Z1*(B-A)+B+A)/TWO
C 10    SUM=SUM+FUNC(VAR1)*DSQRT(ONE-Z1*Z1)
C      AREA=(B-A)*PI*SUM/DFLOAT(2*M)
C
C      RETURN
C      END

```

```

C -----
C      SUBROUTINE CHEB11(FUNC,CON1,AREA,A,B,M)
C
C      PURPOSE: PERFORM INTEGRATION OF F(X) BETWEEN A AND B
C              USING M-POINT GAUSS-CHEBYSHEV QUADRATURE FORMULA
C
C      IMPLICIT REAL*8 (A-H,O-Z)
C      PARAMETER(ZERO=0.0D+00,ONE=1.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
C      PI=FOUR*Datan(ONE)
C      AREA=ZERO
C      SUM=ZERO
C      DO 10 I=1,M
C          Z1=DCOS(DFLOAT(2*(I-1)+1)*PI/DFLOAT(2*M))
C          VAR1=(Z1*(B-A)+B+A)/TWO
C 10    SUM=SUM+FUNC(VAR1,CON1)*DSQRT(ONE-Z1*Z1)
C      AREA=(B-A)*PI*SUM/DFLOAT(2*M)
C
C      RETURN
C      END
C -----
C      SUBROUTINE CHEB12(FUNC,CON1,CON2,AREA,A,B,M)
C
C      PURPOSE: PERFORM INTEGRATION OF F(X) BETWEEN A AND B
C              USING M-POINT GAUSS-CHEBYSHEV QUADRATURE FORMULA
C
C      IMPLICIT REAL*8 (A-H,O-Z)
C      PARAMETER(ZERO=0.0D+00,ONE=1.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
C      PI=FOUR*Datan(ONE)
C      AREA=ZERO
C      SUM=ZERO
C      DO 10 I=1,M
C          Z1=DCOS(DFLOAT(2*(I-1)+1)*PI/DFLOAT(2*M))
C          VAR1=(Z1*(B-A)+B+A)/TWO
C 10    SUM=SUM+FUNC(VAR1,CON1,CON2)*DSQRT(ONE-Z1*Z1)
C      AREA=(B-A)*PI*SUM/DFLOAT(2*M)
C
C      RETURN
C      END
C -----
C      SUBROUTINE CHEB20(FUNC,VAR1,AREA,A,B,M)
C
C      PURPOSE: PERFORM INTEGRATION OF F(X) BETWEEN A AND B
C              USING M-POINT GAUSS-CHEBYSHEV QUADRATURE FORMULA
C
C      IMPLICIT REAL*8 (A-H,O-Z)
C      PARAMETER(ZERO=0.0D+00,ONE=1.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
C      PI=FOUR*Datan(ONE)
C      AREA=ZERO
C      SUM=ZERO
C      DO 10 I=1,M
C          Z1=DCOS(DFLOAT(2*(I-1)+1)*PI/DFLOAT(2*M))
C          VAR2=(Z1*(B-A)+B+A)/TWO
C 10    SUM=SUM+FUNC(VAR1,VAR2)*DSQRT(ONE-Z1*Z1)
C      AREA=(B-A)*PI*SUM/DFLOAT(2*M)
C
C      RETURN
C      END
C -----
C      SUBROUTINE CHEB21(FUNC,VAR1,CON1,AREA,A,B,M)
C
C      PURPOSE: PERFORM INTEGRATION OF F(X) BETWEEN A AND B
C              USING M-POINT GAUSS-CHEBYSHEV QUADRATURE FORMULA
C
C      IMPLICIT REAL*8 (A-H,O-Z)
C      PARAMETER(ZERO=0.0D+00,ONE=1.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
C      PI=FOUR*Datan(ONE)
C      AREA=ZERO
C      SUM=ZERO
C      DO 10 I=1,M
C          Z1=DCOS(DFLOAT(2*(I-1)+1)*PI/DFLOAT(2*M))
C          VAR2=(Z1*(B-A)+B+A)/TWO

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```

10 SUM=SUM+FUNC(VAR1,VAR2,CON1)*DSQRT(ONE-Z1*Z1)
    AREA=(B-A)*PI*SUM/DFLOAT(2*M)
C
C      RETURN
C      END
C
C -----
C      SUBROUTINE CHEB25(FUNC,VAR1,CON1,CON2,CON3,CON4,CON5,AREA,A,B,M)
C
C      PURPOSE: PERFORM INTEGRATION OF F(X) BETWEEN A AND B
C              USING M-POINT GAUSS-CHEBYSHEV QUADRATURE FORMULA
C
C      IMPLICIT REAL*8 (A-H,O-Z)
C      PARAMETER(ZERO=0.0D+00,ONE=1.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
C      PI=FOUR*DATAN(ONE)
C      AREA=ZERO
C      SUM=ZERO
C      DO 10 I=1,M
C          Z1=DCOS(DFLOAT(2*(I-1)+1)*PI/DFLOAT(2*M))
C          VAR2=(Z1*(B-A)+B+A)/TWO
C
10 SUM=SUM+FUNC(VAR1,VAR2,CON1,CON2,CON3,CON4,CON5)*DSQRT(ONE-Z1*Z1)
    AREA=(B-A)*PI*SUM/DFLOAT(2*M)
C
C      RETURN
C      END
C
C -----
C      SUBROUTINE CHEB35(FUNC,VAR1,VAR2,CON1,CON2,CON3,CON4,CON5,AREA,A,B
&,M)
C
C      PURPOSE: PERFORM INTEGRATION OF F(X) BETWEEN A AND B
C              USING M-POINT GAUSS-CHEBYSHEV QUADRATURE FORMULA
C
C      IMPLICIT REAL*8 (A-H,O-Z)
C      PARAMETER(ZERO=0.0D+00,ONE=1.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
C      PI=FOUR*DATAN(ONE)
C      AREA=ZERO
C      SUM=ZERO
C      DO 10 I=1,M
C          Z1=DCOS(DFLOAT(2*(I-1)+1)*PI/DFLOAT(2*M))
C          VAR3=(Z1*(B-A)+B+A)/TWO
C
10 SUM=SUM+FUNC(VAR1,VAR2,VAR3,CON1,CON2,CON3,CON4,CON5)
& *DSQRT(ONE-Z1*Z1)
    AREA=(B-A)*PI*SUM/DFLOAT(2*M)
C
C      RETURN
C      END
FUNCTION ERFC(A)
C
C -----
C      PURPOSE: TO CALCULATE ERFC(A)
C
IMPLICIT REAL*8 (A-H,O-Z)
ERFC=0.0
C=A*A
IF((DABS(C).GT.170.).AND.(A.GE.0.)) RETURN
IF(C.LT.-170.) GO TO 3
X=DABS(A)
IF(X.GT.3.0) GO TO 1
T=1./(1.+.3275911*X)
Y=T*(.2548296-T*(.2844967-T*(1.421414-T*(1.453152-1.061405*T))))*
GO TO 2
1 Y=.5641896/(X+.5/(X+1./(X+1.5/(X+2./(X+2.5/(X+1.))))))
2 ERFC=Y*DEXP(C)
3 IF(A.LT.0.0) ERFC=2.-ERFC
RETURN
END
C
C -----
FUNCTION EXPBIO(X,Z)
IMPLICIT REAL*8(A-Z)

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```

C PURPOSE: TO CALCULATE PRODUCT OF EXP(Z) AND I0(X) (ZERO-ORDER
C MODIFIED BESSEL FUNCTION OF THE FIRST KIND)
C
C DATA P1,P2,P3,P4,P5,P6,P7/1.0D0,3.5156229D0,3.0899424D0,
$ 1.2067492D0,0.2659732D0,0.360768D-1,0.45813D-2/
C DATA Q1,Q2,Q3,Q4,Q5,Q6,Q7,Q8,Q9/0.39894228D0,0.1328592D-1,
$ 0.225319D-2,-0.157565D-2,0.916281D-2,-0.2057706D-1,
$ 0.2635537D-1,-0.1647633D-1,0.392377D-2/
C
C IF (DABS(X).LT.3.75) THEN
Y=(X/3.75)**2
EXPBIO=DEXP(Z)*(P1+Y*(P2+Y*(P3+Y*(P4+Y*(P5+Y*(P6+Y*P7))))))
ELSE
AX=DABS(X)
Y=3.75/AX
EXPBIO=DEXP(AX+Z)/DSQRT(AX)*(Q1+Y*(Q2+Y*(Q3+Y*(Q4+Y*(Q5+Y*
$ (Q6+Y*(Q7+Y*(Q8+Y*Q9)))))))
ENDIF
RETURN
END
C
C -----
FUNCTION EXPBI1(X,Z)
IMPLICIT REAL*8(A-Z)
C
C PURPOSE: TO CALCULATE PRODUCT OF EXP(Z) AND I1(X) (FIRST-ORDER
C MODIFIED BESSEL FUNCTION OF THE FIRST KIND)
C
C DATA P1,P2,P3,P4,P5,P6,P7/0.5D0,0.87890594D0,0.51498869D0,
$ 0.15084984D0,0.2658733D-1,0.301532D-2,0.32411D-3/
C DATA Q1,Q2,Q3,Q4,Q5,Q6,Q7,Q8,Q9/0.39894228D0,-0.3988024D-1,
$ -0.3662018D-2,0.163801D-2,-0.1031555D-1,0.2282967D-1,
$ -0.2895312D-1,0.1787654D-1,-0.420059D-2/
C
C IF (DABS(X).LT.3.75) THEN
Y=(X/3.75)**2
EXPBI1=DEXP(Z)*X*(P1+Y*(P2+Y*(P3+Y*(P4+Y*(P5+Y*(P6+Y*P7))))))
ELSE
AX=DABS(X)
Y=3.75/AX
EXPBI1=DEXP(AX+Z)/DSQRT(AX)*(Q1+Y*(Q2+Y*(Q3+Y*(Q4+Y*(Q5+Y*
$ (Q6+Y*(Q7+Y*(Q8+Y*Q9)))))))
IF(X.LT.0.) EXPBI1=-EXPBI1
ENDIF
RETURN
END
C
C -----
FUNCTION GOLD(X,Y)
C
C PURPOSE: TO CALCULATE GOLDSTEIN'S J-FUNCTION J(X,Y)
C
C IMPLICIT REAL*8(A-H,O-Z)
GOLD=0.0
BF=0.0
E=2.*DSQRT(DMAX1(1.D-35,X*Y))
Z=X+Y-E
IF(Z.GT.17.) GO TO 8
IF(E.GT.1.D-15) GO TO 2
GOLD=DEXP(-X)
RETURN
2 A=DMAX1(X,Y)
B=DMIN1(X,Y)
NT=11.+2.*B+0.3*A
IF(NT.GT.25) GO TO 6
I=0
IF(X.LT.Y) I=1
GXY=1.+I*(B-1.)
GXYO=GXY
GX=1.0

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```

GY=GXY
GZ=1.0
DO 4 K=1,NT
GX=GX*A/K
GY=GY*B/(K+I)
GZ=GZ+GX
GXY=GXY+GY*GZ
IF((GXY-GXYO)/GXY.LT.1.D-08) GO TO 5
4 GXYO=GXY
5 GOLD=GXY*DEXP(-X-Y)
GO TO 8
6 DA=DSQRT(A)
DB=DSQRT(B)
P=3.75/E
B0=(-.3989423+P*(.01328592+P*(.00225319-P*(.00157565-P*(.00916281-P
$*(.02057706-P*(.02635537-P*(.01647633-.00392377*P)))))))/DSQRT(E)
BF=B0*DEXP(-Z)
P=1.+(1.+.3275911*(DA-DB))
ERF=P*(.2548296-P*(.2844967-P*(1.421414-P*(1.453152-P*1.061405))))
P=0.25/E
C0=1.-1.772454*(DA-DB)*ERF
C1=0.5-Z*C0
C2=0.75-Z*C1
C3=1.875-Z*C2
C4=6.5625-Z*C3
SUM=.1994711*(A-B)*P*(C0+1.5*P*(C1+1.666667*P*(C2+1.75*P*(C3+P*(C4
$*(1.8-3.3*P*Z)+97.45313*P)))))
GOLD=0.5*BF+(.3535534*(DA+DB)*ERF+SUM)*BF/(B0*DSQRT(E))
8 IF(X.LT.Y) GOLD=1.+BF-GOLD
RETURN
END
C
C ---
FUNCTION PHI1(TAU)
C
C PURPOSE: TO CALCULATE SERIES IN EXPONENTIAL BVP
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/BVP/ NBP,TOB,DMB,GPB(10),TPB(10),GEB,ALB,JB
PARAMETER(ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00,
& FOUR=4.0D+00)
C
U=ALB-OMU2
IF(ABS(U).LE.ZIP) U=ZIP
PHI1=ZERO
FN=ONE
DO 12 N=1,25
SUMK=ZERO
K=1
CK=ONE
FNK=FN
FN=FN*N
9 CK=-CK
SUMK=SUMK+CK*(X(1)-TAU)**(N-K)/(U**K)/FNK
IF (N.EQ.K) GOTO 12
FNK=FNK/(N-K)
K=K+1
GOTO 9
12 PHI1=PHI1+SUMK*((OMOM*TAU)**N)/FN
C
RETURN
END
C
C ---
FUNCTION PHI2(TAU)
C
C PURPOSE: TO CALCULATE SERIES IN EXPONENTIAL BVP
C

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IMPLICIT REAL*8(A-H,O-Z)
COMMON X(4),R,PX,PY,PZ,BETA,OMEGA,U1,U2,MP,MC,NGC,NP,BINT
COMMON OMU1,OMU2,OM1,OM2,OMOM,U1R,U2R
COMMON/BVP/ NBP,T0B,DMB,GPB(10),TPB(10),GEB,ALB,JB
PARAMETER(ZERO=0.0D+00,ZIP=1.0D-10,ONE=1.0D+00,TWO=2.0D+00,
& FOUR=4.0D+00)
C
      U=ALB-OMU2
      IF(ABS(U).LE.ZIP) U=ZIP
      PHI2=ZERO
      FN=ONE
      DO 12 N=1,25
      SUMK=ZERO
      K=1
      CK=ONE
      FNK=FN
      FN=FN*N
      9   CK=-CK
      SUMK=SUMK+CK*(X(1)-TAU)**(N-K+1)/(U**K)/FNK/(N-K+1)
      IF (N.EQ.K) GOTO 12
      FNK=FNK/(N-K)
      K=K+1
      GOTO 9
12   PHI2=PHI2+SUMK*((OMOM*TAU)**N)/FN
C
      RETURN
      END

```