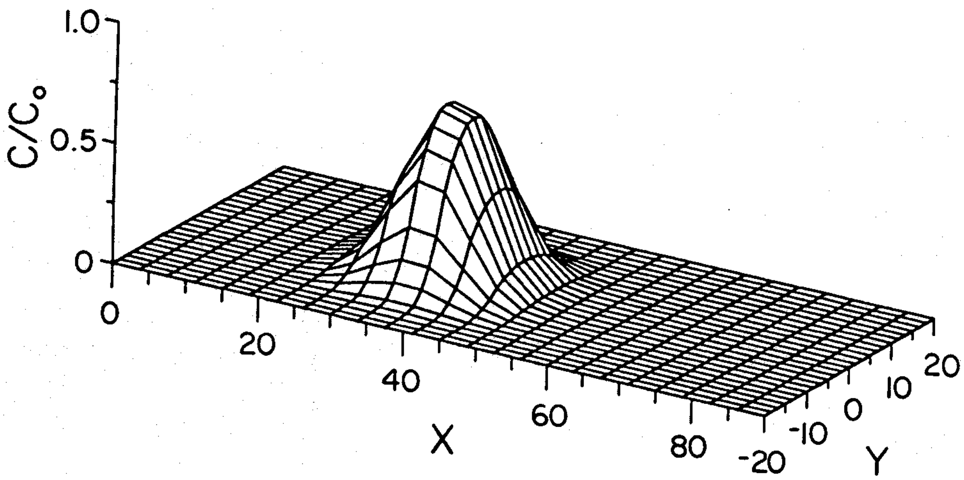
# 3DADE: A COMPUTER PROGRAM FOR EVALUATING THREE-DIMENSIONAL EQUILIBRIUM SOLUTE TRANSPORT IN POROUS MEDIA




Research Report No. 134

May 1994

U. S. SALINITY LABORATORY
AGRICULTURAL RESEARCH SERVICE
U. S. DEPARTMENT OF AGRICULTURE
RIVERSIDE, CALIFORNIA

# 3DADE: A COMPUTER PROGRAM FOR EVALUATING THREE-DIMENSIONAL EQUILIBRIUM SOLUTE TRANSPORT IN POROUS MEDIA

Feike J. Leij and Scott A. Bradford

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# DISCLAIMER

The 3DADE code was developed primarily for research purposes to evaluate analytical solutions published by *Leij et al.* [1991]. The code lacks the versatility to handle a wide variety of transport scenarios, whereas computational efficiency and user-friendliness were not a major concern during code development. The program has been verified for many transport scenarios using a variety of transport parameters. However, no guarantee can be given that the program is completely error-free, or functions according to the intent of all users. Particularly, the use of the nonlinear optimization routine may result in run time errors and nonunique parameter estimates. The 3DADE computer program is a public domain code, which may be used and copied freely. Users are encouraged to communicate their experiences with 3DADE to the authors at the following address

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## ABSTRACT

This research report documents the Fortran program 3DADE (3-Dimensional Advection-Dispersion Equation) for evaluating analytical solutions described in the paper by *Leij et al.* [1991*b*]. The analytical solutions pertain to selected cases of three-dimensional solute transport during steady unidirectional water flow in porous media with uniform transport and flow properties. The transport equation contains terms accounting for solute movement by advection and dispersion, as well as for solute retardation, first-order decay, and zero-order production. The 3DADE code can be used to solve the direct problem, i.e., the concentration is calculated as a function of time and space for specified model parameters, and the indirect (inverse) problem in which the program estimates selected parameters by fitting one of the analytical solutions to specified experimental data. Transient analytical solutions are evaluated for five different transport scenarios (three boundary value problems and two initial value problems) in either a Cartesian or cylindrical coordinate system. Simple steady-state solutions are also provided for three initial value problems. The report contains the main program variables, the input file format, listings of sample input and output files, and a hard copy of the FORTRAN source code.

TABLE OF CONTENTS

# 1. INTRODUCTION

The purpose of the 3DADE code, described in this report, is to evaluate analytical solutions of the three-dimensional advection-dispersion equation for relatively simple transport scenarios in semi-infinite homogeneous porous media presented by *Leij et al.* [1991*b*]. Analytical solutions of subsurface transport problems can be useful: (i) for evaluating the results of numerical solution procedures, (ii) for providing a quick and rough estimate of the solute distribution when the use of numerical methods is not convenient or inaccurate (e.g., over large spatial or temporal scales, and if insufficient information is available to fully describe the mathematical problem), or (iii) for sensitivity analyses to investigate the effect of various transport parameters. The disadvantage of analytical methods, as compared to numerical methods, is that they can only be applied to highly idealized cases [cf. *Javandel et al.* 1984].

Analytical solutions for three-dimensional models exist for both equilibrium [e.g. *Cleary and Ungs*, 1978; *Leij et al.*, 1991*b*] and nonequilibrium transport [*Goltz and Roberts*, 1986; *Leij et al.*, 1993]. Details on the derivation of the solutions for equilibrium transport in either a Cartesian and a cylindrical coordinate system were previously given by *Leij et al.* [1991*b*]. The solutions are used in 3DADE for two purposes. First, the code can be used to solve the *direct* problem by predicting solute concentrations as a function of space and/or time for specified model parameters. Results of 3DADE are, for example, presented in the text by *Ségol* [1994] on the evaluation of numerical models. Second, 3DADE can be used to solve the *indirect* (inverse) problem by fitting selected transport parameters in appropriate analytical solutions to observed solute concentrations. The indirect problem is an extension of the analysis by *Parker and van Genuchten* [1984] of one-dimensional field and laboratory experiments. These authors determined transport parameters using a nonlinear least-squares method based on Marquardt's maximum neighborhood method [*Marquardt*, 1963]. The reliability of the solution for the indirect problem depends on the quality and quantity of the experimental data, correspondence between the experimental conditions in the field or laboratory and the idealized conditions for which the analytical solutions were derived, and sometimes on having reasonable initial estimates for the parameters.

Section 2 of the report will briefly state the boundary and initial conditions for which analytical solutions were obtained, including a graphical illustration of these mathematical conditions, and provide a listing of 13 corresponding solutions. The accuracy of some of the solutions is evaluated in section 3 through comparison with simpler one-dimensional or steady-state solutions. The sensitivity of the solution to the numerical evaluation of the integrals appearing in the analytical solution will also be demonstrated. Section 4 provides a broad outline of the computer program, including the solution of the direct and indirect problems, subroutines for special functions and numerical integration, and the organization of program input and output. Finally, the estimation of model parameters by fitting analytical solutions to observed concentrations is discussed in section 5. Several appendices are included to illustrate input and output files for examples pertaining to both the direct and indirect problems, as well as a listing of 3DADE.

## 2. MATHEMATICAL DESCRIPTION

In order to analytically model solute transport in the subsurface environment, we consider the fairly restrictive case of steady unidirectional (e.g., downward) flow in a porous medium with homogeneous transport properties. In Cartesian coordinates the transport equation can then be written as

$$R\frac{\partial C}{\partial t} = D_x\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} + D_y\frac{\partial^2 C}{\partial y^2} + D_z\frac{\partial^2 C}{\partial z^2} - \mu C + \lambda \tag{1}$$

$$(t > 0,\ 0 \le x < \infty,\ -\infty < y < \infty,\ -\infty < z < \infty)$$

whereas for cylindrical coordinates transport is described with

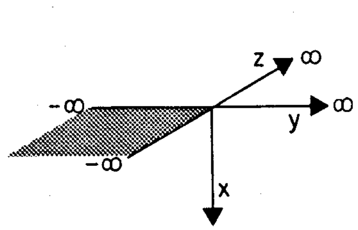
$$R\frac{\partial C}{\partial t} = D_x\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} + \frac{D_r}{r}\frac{\partial}{\partial r}\left[r\frac{\partial C}{\partial r}\right] - \mu C + \lambda \tag{2}$$

$$(t > 0,\quad 0 \le x < \infty,\ 0 < r < \infty)$$

where $R$ is the retardation factor; $C$ is the volume-averaged or resident concentration of the solute ($ML^{-3}$); $t$ is time (T); $x$ is the position (L) in the direction of flow; $y$ and $z$ are rectangular coordinates and $r$ is a cylindrical coordinate, all three are perpendicular to the flow direction (L); $D_x$, $D_y$, $D_z$, and $D_r$ are dispersion coefficients ($L^2T^{-1}$) in the $x$, $y$, $z$, and $r$ directions, respectively; $v$ is the pore-water velocity ($LT^{-1}$); $\mu$ is a first-order rate coefficient for decay ($T^{-1}$); and $\lambda$ is a general zero-order rate coefficient for production ($ML^{-3}T^{-1}$).

The initial and input concentrations for five scenarios for which solutions were derived by *Leij et al.* [1991] are given in Fig. 1. Scenarios 1, 2, and 3 concern a Cartesian or rectangular coordinate system, whereas scenarios 4 and 5 involve cylindrical coordinates. Furthermore, a distinction is made between a boundary value problem (scenarios 1, 2, and 4) and an initial value problem (scenarios 3 and 5). For boundary value problems 1, 2, and 4, the surface area from which the solute is applied between times 0 and $t_o$ is shaded in Fig. 1. For initial value problems 3 and 5, $C_o$ denotes the uniform initial concentration in the rectangular and cylindrical volume, respectively. Each case was solved for a first-type inlet condition, i.e., a continuous concentration at the inlet:

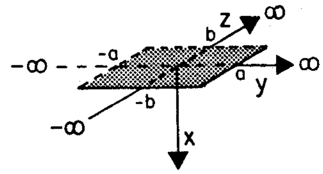
1




$$g(y,z,t) = \begin{cases} C_o & y<0, z<0, 0<t\le t_o \\ 0 & \text{otherwise} \end{cases}$$

$$C(x,y,z,0) = 0$$

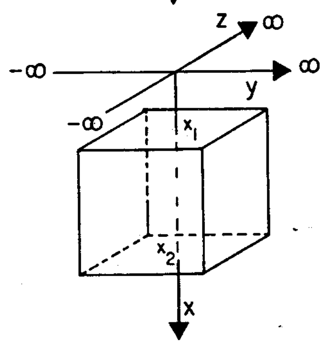
2




$$g(y,z,t) = \begin{cases} C_o & |y|<a, |z|<b, 0<t\le t_o \\ 0 & \text{otherwise} \end{cases}$$

$$C(x,y,z,0) = 0$$

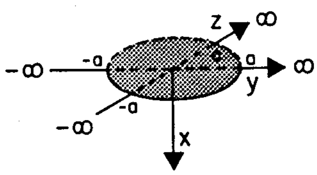
3




$$g(y,z,t) = 0$$

$$C(x,y,z,0) = \begin{cases} C_o & x_1<x<x_2, |y|<a, |z|<b \\ 0 & \text{otherwise} \end{cases}$$

4

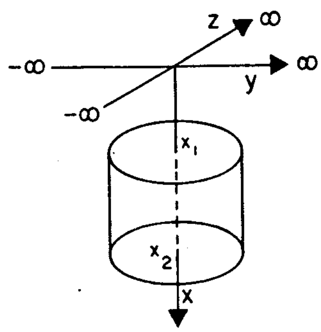



$$g(r,t) = \begin{cases} C_o & r<a, 0<t\le t_o \\ 0 & \text{otherwise} \end{cases}$$

$$C(x,r,0) = 0$$

$$r = \sqrt{y^2+z^2}$$

5




$$g(r,t) = 0$$

$$C(x,r,0) = \begin{cases} C_o & x_1<x<x_2, r<a \\ 0 & \text{otherwise} \end{cases}$$

$$r = \sqrt{y^2+z^2}$$

Fig. 1. Schematic of inlet and initial distributions for: (1) diffuse source in semi-infinite region of surface, (2) rectangular source at surface, (3) parallelepipedal initial distribution, (4) circular source at surface, and (5) cylindrical initial distribution.

$$C(x,y,z,t)\,|_{x=0^+} = g(y,z,t) \quad \text{or} \quad C(x,r,t)\,|_{x=0^+} = g(r,t) \tag{3}$$

and a third-type boundary condition:

$$\left(C - \frac{D_x}{v}\frac{\partial C}{\partial x}\right)\Big|_{x=0^+} = g(y,z,t) \text{ or } g(r,t) \tag{4}$$

where the input concentration $g$ is a pulse with concentration $C_o$ of duration $t_o$ for scenarios 1, 2, and 4. The outlet condition is given by

$$\frac{\partial C}{\partial x}\Big|_{x\to\infty} = 0 \tag{5}$$

*Van Genuchten and Parker* [1984] have demonstrated that a third-type inlet condition should be used for resident concentrations to ensure mass conservation. Many solute displacement experiments involve the determination of flowing or flux-averaged concentrations. Flux-averaged concentrations represent the ratio of the solute flux to the water flux. They are typically observed for effluent samples obtained from experiments involving laboratory columns or sand boxes, and they may also be encountered for injection and observation wells in the field. Calculated concentrations can be made consistent with observed effluent concentrations by employing the well known transformation from resident ($C_R$) to flux-averaged ($C_F$) concentrations [*Kreft and Zuber*, 1978]:

$$C_F = C_R - \frac{D_x}{v}\frac{\partial C_R}{\partial x} \tag{6}$$

When the initial distribution is uniform (e.g. scenarios 1, 2, and 4), it can be shown with Eq. (6) that the use of a third-type inlet condition for transport problems in terms of resident concentrations, is mathematically equivalent to the use of a first-type inlet condition in conjunction with flux-averaged concentrations. If the initial distribution is nonuniform, however, this equivalence does not hold because the initial condition formulated in terms of $C_R$ will be different from the initial distribution in terms of $C_F$. In this case, expressions for $C_F$ can be derived by transforming the *solutions* for $C_R$, obtained for a third-type inlet condition, according to Eq.(6) [cf. *Toride et al.,* 1993*a*].

The principle of superposition may be applied to the initial and boundary value problems because of linearity of the transport problem. For instance, if solute is applied to an area depicted in scenario 2, of a medium with an initial distribution according to scenario 3, the solute concentration in the soil can be predicted by summing up the solutions to the separate (homogeneous) boundary and initial value problems [cf. *Toride et al.*, 1993*b*].

The multidimensional transport problems were solved with the help of integral transforms as outlined by *Leij et al.* [1991*b*]. The solutions are listed in Table 1 for the five transient scenarios of Fig. 1 using a first- or third-type inlet condition (F or T) and three steady-state solutions (SS). The meaning of the variables $x_1$, $x_2$, $a$, and $b$ follows from Fig. 1. All parameters should be expressed in consistent units; the user can select an arbitrary unit for each dimension. Note that if $C_o$ is set to unity, the predicted concentration is in effect dimensionless. The solutions in the Cartesian coordinate system can be readily adopted for two-dimensional transport, for instance, by assuming $z \to -\infty$ in scenario 1 or $b \to \infty$ in scenarios 2 and 3. As mentioned, the solutions can be applied to describe transport in cases where solute is applied to a medium with a nonzero initial distribution using the principle of superposition. The program also includes three simple steady-state solutions for continuous solute application according to scenarios 1, 2, and 4, i.e., $t_o$ is infinite, with no production and decay processes ($\mu = \lambda = 0$). For convenience, we have assumed that for the steady state solution longitudinal dispersion can be ignored because of its minor influence compared to other transport processes [*Harleman and Rumer*, 1963]. In this case the first- and third-type inlet conditions are identical. Because solute retardation does not influence the steady-state solute distribution, the value for $R$ can also be ignored. The steady-state solutions are given in Table 1 as well.

The complementary error function (erfc) was programmed according to *van Genuchten and Alves* [1982] whereas the zero-order modified Bessel function ($I_0$) was obtained with the program from *Press et al.* [1986]. The integrals in these solutions are evaluated using Gauss-Chebyshev quadrature as outlined by *Leij et al.* [1991*a*]. For integration with respect to $\tau$ for the interval $[\alpha,\beta]$, first, the standard linear transformation $\tau = [(\alpha-\beta)\eta + \alpha + \beta]/2$ is used to change the integration limits. Subsequently, the Gauss-Chebyshev formula yields

$$\int_{\alpha}^{\beta} f(\tau)\, d\tau = \frac{\gamma_k(\alpha-\beta)}{2} \sum_{k=1}^{n} \sqrt{(1-\eta_k^2)}\; f\{[(\beta-\alpha)\eta_k + (\beta+\alpha)]/2\} \tag{7}$$

where the roots and coefficients are given by

$$\eta_k = \cos[\frac{(2k-1)\pi}{2n}] \quad \text{and} \quad \gamma_k = \pi/n \qquad\qquad k = 1,2,,....,n$$

Both single and multiple integrations are conveniently carried out with the subroutine described by *Carnahan et al.* [1969]. The accuracy of the approximation depends on the value for $n$, the number of Gauss-Chebyshev points (NGC).

Table 1. Analytical Expressions for $C(x,y,z,t)$ or $C(x,r,t)$

| *Model-Scenario* | *Solution*† |
| --- | --- |
| 1-F1 | $\frac{C_o}{4}\int_{P(t)}^{t} \Lambda_1(\tau)\Gamma_1(\tau)d\tau + \frac{\lambda}{2R}\int_0^t \Lambda_2(\tau)d\tau$ |
| 2-T1 | $\frac{C_o}{4}\int_{P(t)}^{t} \frac{v}{R}\Lambda_3(\tau)\Gamma_1(\tau)d\tau + \frac{\lambda}{2R}\int_0^t \Lambda_4(\tau)d\tau$ |
| 3-F2 | $\frac{C_o}{4}\int_{P(t)}^{t} \Lambda_1(\tau)\Gamma_2(\tau)d\tau + \frac{\lambda}{2R}\int_0^t \Lambda_2(\tau)d\tau$ |
| 4-T2 | $\frac{C_o}{4}\int_{P(t)}^{t} \frac{v}{R}\Lambda_3(\tau)\Gamma_2(\tau)d\tau + \frac{\lambda}{2R}\int_0^t \Lambda_4(\tau)d\tau$ |
| 5-F3 | $\frac{C_o}{8}\Lambda_5(t)\Gamma_2(t) + \frac{\lambda}{2R}\int_0^t \Lambda_2(\tau)d\tau$ |
| 6-T3 | $\frac{C_o}{8}\Lambda_6(t)\Gamma_2(t) + \frac{\lambda}{2R}\int_0^t \Lambda_4(\tau)d\tau$ |
| 7-F4 | $\frac{C_o}{2}\int_{P(t)}^{t}\int_0^a \Lambda_1(\tau)\Xi(\rho,\tau)d\rho\, d\tau + \frac{\lambda}{2R}\int_0^t \Lambda_2(\tau)\, d\tau$ |
| 8-T4 | $\frac{C_o}{2}\int_{P(t)}^{t}\int_0^a \frac{v}{R}\Lambda_3(\tau)\Xi(\rho,\tau)d\rho\, d\tau + \frac{\lambda}{2R}\int_0^t \Lambda_4(\tau)\, d\tau$ |
| 9-F5 | $\frac{C_o}{4}\int_0^a \Lambda_5(t)\Xi(\rho,t)d\rho + \frac{\lambda}{2R}\int_0^\infty \Lambda_2(\tau)\, d\tau$ |
| 10-T5 | $\frac{C_o}{4}\int_0^a \Lambda_6(t)\Xi(\rho,t)d\rho + \frac{\lambda}{2R}\int_0^t \Lambda_4(\tau)\, d\tau$ |
| 11-SS1 | $\frac{C_o}{4}\mathrm{erfc}\left[\frac{y}{(4D_y x/v)^{1/2}}\right]\mathrm{erfc}\left[\frac{z}{(4D_z x/v)^{1/2}}\right]$ |
| 12-SS2 | $\frac{C_o}{4}\left[\mathrm{erfc}\left(\frac{y-a}{(4D_y x/v)^{1/2}}\right) - \mathrm{erfc}\left(\frac{y+a}{(4D_y x/v)^{1/2}}\right)\right]\left[\mathrm{erfc}\left(\frac{z-b}{(4D_z x/v)^{1/2}}\right) - \mathrm{erfc}\left(\frac{z+b}{(4D_z x/v)^{1/2}}\right)\right]$ |
| 13-SS4 | $\int_0^a \frac{v\rho C_o}{2D_r x}\exp\left(-\frac{v(r^2+\rho^2)}{4D_r x}\right) \mathrm{I}_0\left(\frac{vr\rho}{2D_r x}\right) d\rho$ |

† $P(t)=0$ if $0<t\leq t_o$ and $t-t_o$ if $t>t_o$

Table 1. (Continued)

$$\Gamma_1(\tau) = \operatorname{erfc}\left[\frac{y}{(4D_y\tau/R)^{1/2}}\right] \operatorname{erfc}\left[\frac{z}{(4D_z\tau/R)^{1/2}}\right]$$

$$\Gamma_2(\tau) = \left[\operatorname{erfc}\left(\frac{y-a}{(4D_y\tau/R)^{1/2}}\right) - \operatorname{erfc}\left(\frac{y+a}{(4D_y\tau/R)^{1/2}}\right)\right]\left[\operatorname{erfc}\left(\frac{z-b}{(4D_z\tau/R)^{1/2}}\right) - \operatorname{erfc}\left(\frac{z+b}{(4D_z\tau/R)^{1/2}}\right)\right]$$

$$\Xi(\rho,\tau) = \frac{\rho R}{D_r\tau}\exp\left(-\frac{R(r^2+\rho^2)}{(4D_r\tau)}\right) I_0\left(\frac{Rr\rho}{2D_r\tau}\right)$$

$$\Lambda_1(\tau) = \left(\frac{Rx^2}{4\pi D_x\tau^3}\right)^{1/2}\exp\left(-\frac{\mu\tau}{R}-\frac{(Rx-v\tau)^2}{4RD_x\tau}\right)$$

$$\Lambda_2(\tau) = \exp\left(-\frac{\mu\tau}{R}\right)\left[\operatorname{erfc}\left(\frac{v\tau-Rx}{(4RD_x\tau)^{1/2}}\right) - \exp\left(\frac{vx}{D_x}\right)\operatorname{erfc}\left(\frac{Rx+v\tau}{(4RD_x\tau)^{1/2}}\right)\right]$$

$$\Lambda_3(\tau) = \exp\left(-\frac{\mu\tau}{R}\right)\left[\left(\frac{R}{\pi D_x\tau}\right)^{1/2}\exp\left(-\frac{(Rx-v\tau)^2}{4RD_x\tau}\right) - \frac{v}{2D_x}\exp\left(\frac{vx}{D_x}\right)\operatorname{erfc}\left(\frac{Rx+v\tau}{(4RD_x\tau)^{1/2}}\right)\right]$$

$$\Lambda_4(\tau) = \exp\left(-\frac{\mu\tau}{R}\right)\left[\operatorname{erfc}\left(\frac{v\tau-Rx}{(4RD_x\tau)^{1/2}}\right) + \left(1+\frac{v}{D_x}(x+v\tau/R)\right)\exp\left(\frac{vx}{D_x}\right)\operatorname{erfc}\left(\frac{Rx+v\tau}{(4RD_x\tau)^{1/2}}\right) - \left(\frac{4v^2\tau}{\pi RD_x}\right)^{1/2}\exp\left(-\frac{(Rx-v\tau)^2}{4RD_x\tau}\right)\right]$$

$$\Lambda_5(t) = \exp\left(-\frac{\mu t}{R}\right)\left\{\operatorname{erfc}\left(\frac{R(x-x_2)-vt}{(4RD_xt)^{1/2}}\right) - \operatorname{erfc}\left(\frac{R(x-x_1)-vt}{(4RD_xt)^{1/2}}\right) + \exp\left(\frac{vx}{D_x}\right)\left[\operatorname{erfc}\left(\frac{R(x+x_2)+vt}{(4RD_xt)^{1/2}}\right) - \operatorname{erfc}\left(\frac{R(x+x_1)+vt}{(4RD_xt)^{1/2}}\right)\right]\right\}$$

$$\begin{aligned}\Lambda_6(t) = \exp\left(-\frac{\mu t}{R}\right)\Bigg\{&\exp\left(\frac{vx}{D_x}\right)\left[\left(1+\frac{v}{D_x}(x+x_1+vt/R)\right)\operatorname{erfc}\left(\frac{R(x+x_1)+vt}{(4RD_xt)^{1/2}}\right)\right.\\ &\left.-\left(1+\frac{v}{D_x}(x+x_2+vt/R)\right)\operatorname{erfc}\left(\frac{R(x+x_2)+vt}{(4RD_xt)^{1/2}}\right)\right]\\ &+\operatorname{erfc}\left(\frac{R(x-x_2)-vt}{(4RD_xt)^{1/2}}\right) - \operatorname{erfc}\left(\frac{R(x-x_1)-vt}{(4RD_xt)^{1/2}}\right)\\ &+\left(\frac{4v^2t}{\pi RD_x}\right)^{1/2}\exp\left(\frac{vx}{D_x}\right)\left[\exp\left(-\frac{[R(x+x_2)+vt]^2}{4RD_xt}\right) - \exp\left(-\frac{[R(x+x_1)+vt]^2}{4RD_xt}\right)\right]\Bigg\}\end{aligned}$$

## 3. EVALUATION OF RESULTS

The results of the numerical integration using Gauss-Chebyshev quadrature will generally improve if the number of integration points, NGC, is increased. On the other hand, the solution of both the direct and the indirect problem requires more time if NGC is increased, particularly if multiple integrals are evaluated. To assess the influence of NGC on the predicted concentration, we calculated solute profiles for four examples using several different values for NGC. Furthermore, the results for the transient multi-dimensional solutions will be compared with simpler one-dimensional and steady-state solutions to check the analytical derivation and coding of our solutions.

Table 2 gives predicted solute concentrations versus depth and time, with NGC equal to 10, 25, 50, 100, 200, and 400, for scenario 1 using a first-type inlet condition. Solute was applied to the area of the soil surface given by $y<0$ and $z<0$. An apparent one-dimensional problem was obtained by setting $y=-20$ and $z=-20$ for $0<x<20$. The predicted values for $C/C_o$ appear erroneous if NGC=10 and somewhat unrealistic when NGC=25, whereas for the remaining NGC values the concentration profiles are very similar. The last column provides the concentration according to one-dimensional solution A1 of *van Genuchten and Alves* [1982]. The one- and three-dimensional solutions agree quite well for NGC>50.

Table 3 contains calculated $C(x,t)/C_o$ profiles for scenario 3, i.e., the application of solute-free water to a soil where a solute is initially distributed uniformly between $x=0$ and $x=10$, and where zero- and first-order rate processes are taking place. The problem was again essentially one-dimensional and predictions were made with three-dimensional solution F3 from Table 1, assuming a first-type inlet condition and using NGC values of 10, 20, 30, 40, 50, and 100, and with one-dimensional solution A5 of *van Genuchten and Alves* [1982]. The agreement between the one- and three-dimensional solutions is quite good. Because numerical integration is only required for the production-part of the solution, the use of different NGC values leads only to minor changes in the predicted $C(x,t)$ profiles. Note that for small values of $\mu$ the multi-dimensional solution, with numerical integration, is to be preferred over the one-dimensional solution which contains $\mu$ in the denominator.

Table 2. Solute transport with $v$=50, $R$=1, $t_o$=10, $\mu$=0, $\lambda$=0, $D_x$=50, $D_y$=10, and $D_z$=10 according to scenario 1 for a first-type inlet condition calculated with three-dimensional (**3D**) solution F1 of Table 1 at $y$=-20 and $z$=-20, using various values of NGC, and the one-dimensional (**1D**) solution A1 of *van Genuchten and Alves* [1982]

| | | 3D with NGC= | | | | | | 1D |
|---|---|---|---|---|---|---|---|---|
| | | 10 | 25 | 50 | 100 | 200 | 400 | |
| $t$ | $x$ | $C/C_o$ | | | | | | |
| 0.20 | 2.00 | 1.0183 | 0.9905 | 0.9901 | 0.9901 | 0.9901 | 0.9901 | 0.9901 |
| 0.20 | 4.00 | 0.9572 | 0.9578 | 0.9578 | 0.9578 | 0.9578 | 0.9578 | 0.9578 |
| 0.20 | 6.00 | 0.8846 | 0.8845 | 0.8844 | 0.8844 | 0.8844 | 0.8844 | 0.8844 |
| 0.20 | 8.00 | 0.7590 | 0.7578 | 0.7576 | 0.7576 | 0.7576 | 0.7576 | 0.7576 |
| 0.20 | 10.00 | 0.5871 | 0.5856 | 0.5854 | 0.5853 | 0.5853 | 0.5853 | 0.5853 |
| 0.20 | 12.00 | 0.4000 | 0.3983 | 0.3981 | 0.3980 | 0.3980 | 0.3980 | 0.3980 |
| 0.20 | 14.00 | 0.2355 | 0.2341 | 0.2339 | 0.2338 | 0.2338 | 0.2338 | 0.2338 |
| 0.20 | 16.00 | 0.1182 | 0.1172 | 0.1170 | 0.1170 | 0.1170 | 0.1170 | 0.1170 |
| 0.20 | 18.00 | 0.0501 | 0.0495 | 0.0494 | 0.0494 | 0.0494 | 0.0494 | 0.0494 |
| 0.20 | 20.00 | 0.0178 | 0.0175 | 0.0175 | 0.0175 | 0.0175 | 0.0175 | 0.0175 |
| 0.40 | 2.00 | 0.9236 | 0.9966 | 0.9997 | 0.9996 | 0.9996 | 0.9996 | 0.9996 |
| 0.40 | 4.00 | 0.9990 | 0.9983 | 0.9983 | 0.9983 | 0.9983 | 0.9983 | 0.9983 |
| 0.40 | 6.00 | 0.9957 | 0.9945 | 0.9945 | 0.9945 | 0.9945 | 0.9945 | 0.9945 |
| 0.40 | 8.00 | 0.9856 | 0.9854 | 0.9853 | 0.9853 | 0.9853 | 0.9853 | 0.9853 |
| 0.40 | 10.00 | 0.9661 | 0.9663 | 0.9662 | 0.9662 | 0.9662 | 0.9662 | 0.9662 |
| 0.40 | 12.00 | 0.9323 | 0.9313 | 0.9313 | 0.9312 | 0.9312 | 0.9312 | 0.9312 |
| 0.40 | 14.00 | 0.8754 | 0.8746 | 0.8745 | 0.8744 | 0.8744 | 0.8744 | 0.8744 |
| 0.40 | 16.00 | 0.7939 | 0.7925 | 0.7923 | 0.7922 | 0.7922 | 0.7922 | 0.7922 |
| 0.40 | 18.00 | 0.6879 | 0.6860 | 0.6857 | 0.6856 | 0.6856 | 0.6856 | 0.6856 |
| 0.40 | 20.00 | 0.5642 | 0.5620 | 0.5617 | 0.5616 | 0.5616 | 0.5616 | 0.5616 |
| 0.60 | 2.00 | 0.8128 | 0.9976 | 0.9999 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| 0.60 | 4.00 | 1.0477 | 0.9997 | 0.9999 | 0.9999 | 0.9999 | 0.9999 | 0.9999 |
| 0.60 | 6.00 | 0.9801 | 0.9997 | 0.9997 | 0.9997 | 0.9997 | 0.9997 | 0.9997 |
| 0.60 | 8.00 | 1.0058 | 0.9991 | 0.9991 | 0.9991 | 0.9991 | 0.9991 | 0.9991 |
| 0.60 | 10.00 | 0.9980 | 0.9978 | 0.9978 | 0.9978 | 0.9978 | 0.9978 | 0.9978 |
| 0.60 | 12.00 | 0.9926 | 0.9947 | 0.9947 | 0.9947 | 0.9947 | 0.9947 | 0.9947 |
| 0.60 | 14.00 | 0.9899 | 0.9887 | 0.9887 | 0.9886 | 0.9886 | 0.9886 | 0.9886 |
| 0.60 | 16.00 | 0.9780 | 0.9775 | 0.9774 | 0.9774 | 0.9774 | 0.9774 | 0.9774 |
| 0.60 | 18.00 | 0.9584 | 0.9583 | 0.9583 | 0.9583 | 0.9583 | 0.9583 | 0.9583 |
| 0.60 | 20.00 | 0.9288 | 0.9281 | 0.9279 | 0.9279 | 0.9279 | 0.9279 | 0.9279 |
| 0.80 | 2.00 | 0.8081 | 1.0103 | 1.0004 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| 0.80 | 4.00 | 1.0577 | 1.0010 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| 0.80 | 6.00 | 0.9932 | 1.0001 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| 0.80 | 8.00 | 0.9863 | 0.9999 | 0.9999 | 0.9999 | 0.9999 | 0.9999 | 0.9999 |
| 0.80 | 10.00 | 1.0120 | 0.9999 | 0.9999 | 0.9999 | 0.9999 | 0.9999 | 0.9999 |
| 0.80 | 12.00 | 0.9987 | 0.9996 | 0.9996 | 0.9996 | 0.9996 | 0.9996 | 0.9996 |
| 0.80 | 14.00 | 0.9945 | 0.9991 | 0.9991 | 0.9991 | 0.9991 | 0.9991 | 0.9991 |
| 0.80 | 16.00 | 0.9994 | 0.9981 | 0.9981 | 0.9981 | 0.9981 | 0.9981 | 0.9981 |
| 0.80 | 18.00 | 0.9979 | 0.9960 | 0.9960 | 0.9960 | 0.9960 | 0.9960 | 0.9960 |
| 0.80 | 20.00 | 0.9917 | 0.9921 | 0.9921 | 0.9921 | 0.9921 | 0.9921 | 0.9921 |
| 1.00 | 4.00 | 1.0192 | 1.0018 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| 1.00 | 8.00 | 0.9631 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| 1.00 | 12.00 | 1.0156 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| 1.00 | 16.00 | 0.9921 | 0.9998 | 0.9998 | 0.9998 | 0.9998 | 0.9998 | 0.9998 |
| 1.00 | 20.00 | 1.0036 | 0.9993 | 0.9993 | 0.9993 | 0.9993 | 0.9993 | 0.9993 |

Table 3. Solute transport with $v=20$, $R=1$, $\mu=0.25$, $\lambda=0.10$, $D_x=40$, $D_y=10$, and $D_z=10$ calculated with three-dimensional (3D) solution F3 of Table 1 at $y=0$ and $z=0$, with $a=b=100$, $x_1=0$, and $x_2=10$, using various values of NGC, and with one-dimensional (1D) solution A5 of *van Genuchten and Alves* [1982]

| | | 3D with NGC= | | | | | | 1D |
|---|---|---|---|---|---|---|---|---|
| | | 10 | 20 | 30 | 40 | 50 | 100 | |
| $t$ | $x$ | $C/C_o$ | | | | | | |
| 0.50 | 2.00 | 0.0294 | 0.0294 | 0.0294 | 0.0294 | 0.0294 | 0.0294 | 0.0294 |
| 0.50 | 4.00 | 0.0768 | 0.0767 | 0.0767 | 0.0767 | 0.0767 | 0.0767 | 0.0767 |
| 0.50 | 6.00 | 0.1451 | 0.1450 | 0.1450 | 0.1450 | 0.1450 | 0.1450 | 0.1450 |
| 0.50 | 8.00 | 0.2313 | 0.2312 | 0.2312 | 0.2312 | 0.2312 | 0.2312 | 0.2312 |
| 0.50 | 10.00 | 0.3252 | 0.3251 | 0.3251 | 0.3251 | 0.3251 | 0.3251 | 0.3251 |
| 0.50 | 12.00 | 0.4106 | 0.4105 | 0.4105 | 0.4105 | 0.4105 | 0.4105 | 0.4105 |
| 0.50 | 14.00 | 0.4703 | 0.4702 | 0.4702 | 0.4701 | 0.4701 | 0.4701 | 0.4701 |
| 0.50 | 16.00 | 0.4918 | 0.4916 | 0.4916 | 0.4916 | 0.4916 | 0.4916 | 0.4916 |
| 0.50 | 18.00 | 0.4718 | 0.4717 | 0.4716 | 0.4716 | 0.4716 | 0.4716 | 0.4716 |
| 0.50 | 20.00 | 0.4172 | 0.4171 | 0.4171 | 0.4170 | 0.4170 | 0.4170 | 0.4170 |
| 1.00 | 2.00 | 0.0120 | 0.0118 | 0.0118 | 0.0118 | 0.0118 | 0.0117 | 0.0117 |
| 1.00 | 4.00 | 0.0257 | 0.0256 | 0.0256 | 0.0256 | 0.0255 | 0.0255 | 0.0255 |
| 1.00 | 6.00 | 0.0428 | 0.0426 | 0.0426 | 0.0426 | 0.0426 | 0.0426 | 0.0426 |
| 1.00 | 8.00 | 0.0644 | 0.0642 | 0.0642 | 0.0642 | 0.0642 | 0.0642 | 0.0642 |
| 1.00 | 10.00 | 0.0917 | 0.0915 | 0.0915 | 0.0915 | 0.0915 | 0.0915 | 0.0915 |
| 1.00 | 12.00 | 0.1253 | 0.1251 | 0.1251 | 0.1250 | 0.1250 | 0.1250 | 0.1250 |
| 1.00 | 14.00 | 0.1646 | 0.1645 | 0.1644 | 0.1644 | 0.1644 | 0.1644 | 0.1644 |
| 1.00 | 16.00 | 0.2082 | 0.2081 | 0.2080 | 0.2080 | 0.2080 | 0.2080 | 0.2080 |
| 1.00 | 18.00 | 0.2531 | 0.2529 | 0.2529 | 0.2529 | 0.2529 | 0.2529 | 0.2529 |
| 1.00 | 20.00 | 0.2953 | 0.2951 | 0.2951 | 0.2951 | 0.2951 | 0.2951 | 0.2951 |
| 1.50 | 2.00 | 0.0104 | 0.0100 | 0.0100 | 0.0100 | 0.0100 | 0.0100 | 0.0100 |
| 1.50 | 4.00 | 0.0203 | 0.0201 | 0.0201 | 0.0200 | 0.0200 | 0.0200 | 0.0200 |
| 1.50 | 6.00 | 0.0308 | 0.0305 | 0.0305 | 0.0305 | 0.0305 | 0.0305 | 0.0305 |
| 1.50 | 8.00 | 0.0419 | 0.0417 | 0.0416 | 0.0416 | 0.0416 | 0.0416 | 0.0416 |
| 1.50 | 10.00 | 0.0541 | 0.0539 | 0.0538 | 0.0538 | 0.0538 | 0.0538 | 0.0538 |
| 1.50 | 12.00 | 0.0679 | 0.0677 | 0.0676 | 0.0676 | 0.0676 | 0.0676 | 0.0676 |
| 1.50 | 14.00 | 0.0838 | 0.0836 | 0.0835 | 0.0835 | 0.0835 | 0.0835 | 0.0835 |
| 1.50 | 16.00 | 0.1022 | 0.1019 | 0.1019 | 0.1019 | 0.1018 | 0.1018 | 0.1018 |
| 1.50 | 18.00 | 0.1233 | 0.1231 | 0.1230 | 0.1230 | 0.1230 | 0.1230 | 0.1230 |
| 1.50 | 20.00 | 0.1472 | 0.1469 | 0.1469 | 0.1469 | 0.1469 | 0.1469 | 0.1469 |
| 2.00 | 2.00 | 0.0104 | 0.0098 | 0.0097 | 0.0097 | 0.0097 | 0.0097 | 0.0097 |
| 2.00 | 4.00 | 0.0195 | 0.0193 | 0.0193 | 0.0192 | 0.0192 | 0.0192 | 0.0192 |
| 2.00 | 6.00 | 0.0291 | 0.0287 | 0.0287 | 0.0287 | 0.0286 | 0.0286 | 0.0286 |
| 2.00 | 8.00 | 0.0384 | 0.0381 | 0.0380 | 0.0380 | 0.0380 | 0.0380 | 0.0380 |
| 2.00 | 10.00 | 0.0478 | 0.0475 | 0.0474 | 0.0474 | 0.0474 | 0.0474 | 0.0474 |
| 2.00 | 12.00 | 0.0574 | 0.0571 | 0.0571 | 0.0570 | 0.0570 | 0.0570 | 0.0570 |
| 2.00 | 14.00 | 0.0674 | 0.0671 | 0.0670 | 0.0670 | 0.0670 | 0.0670 | 0.0670 |
| 2.00 | 16.00 | 0.0780 | 0.0776 | 0.0776 | 0.0776 | 0.0775 | 0.0775 | 0.0775 |
| 2.00 | 18.00 | 0.0893 | 0.0890 | 0.0889 | 0.0889 | 0.0889 | 0.0889 | 0.0889 |
| 2.00 | 20.00 | 0.1017 | 0.1014 | 0.1013 | 0.1013 | 0.1013 | 0.1013 | 0.1013 |

Table 4. Transport with $v=20$, $R=1$, $t_o=10$, $\mu=0$, $\lambda=0$, $D_x=5$, $D_y=20$, and $D_z=10$ according to scenario 2 at $x=10$ with $a=10$ and $b=5$, for a third-type inlet condition calculated with **transient** solution T2, using various NGC, and **steady-state** solution SS2 of Table 1

| | | | **Transient with NGC=** | | | | | | **Steady state** |
|---|---|---|---|---|---|---|---|---|---|
| | | | 10 | 20 | 30 | 40 | 50 | 100 | |
| $t$ | $y$ | $z$ | $C/C_o$ | | | | | | |
| 1.00 | 0.00 | 0.00 | 0.8618 | 0.8576 | 0.8576 | 0.8576 | 0.8576 | 0.8576 | |
| 1.00 | 0.00 | 4.00 | 0.6064 | 0.6036 | 0.6036 | 0.6036 | 0.6036 | 0.6036 | |
| 1.00 | 0.00 | 8.00 | 0.1665 | 0.1657 | 0.1657 | 0.1657 | 0.1657 | 0.1657 | |
| 1.00 | 0.00 | 12.00 | 0.0146 | 0.0146 | 0.0146 | 0.0146 | 0.0146 | 0.0146 | |
| 1.00 | 0.00 | 16.00 | 0.0005 | 0.0005 | 0.0005 | 0.0005 | 0.0005 | 0.0005 | |
| 1.00 | 4.00 | 0.00 | 0.8057 | 0.8019 | 0.8019 | 0.8019 | 0.8019 | 0.8019 | |
| 1.00 | 4.00 | 4.00 | 0.5669 | 0.5643 | 0.5643 | 0.5643 | 0.5643 | 0.5643 | |
| 1.00 | 4.00 | 8.00 | 0.1553 | 0.1547 | 0.1547 | 0.1547 | 0.1547 | 0.1547 | |
| 1.00 | 4.00 | 12.00 | 0.0135 | 0.0135 | 0.0135 | 0.0135 | 0.0135 | 0.0135 | |
| 1.00 | 4.00 | 16.00 | 0.0004 | 0.0004 | 0.0004 | 0.0004 | 0.0004 | 0.0004 | |
| 1.00 | 8.00 | 0.00 | 0.5975 | 0.5948 | 0.5948 | 0.5948 | 0.5948 | 0.5948 | |
| 1.00 | 8.00 | 4.00 | 0.4204 | 0.4186 | 0.4186 | 0.4186 | 0.4186 | 0.4186 | |
| 1.00 | 8.00 | 8.00 | 0.1152 | 0.1147 | 0.1147 | 0.1147 | 0.1147 | 0.1147 | |
| 1.00 | 8.00 | 12.00 | 0.0101 | 0.0101 | 0.0101 | 0.0101 | 0.0101 | 0.0101 | |
| 1.00 | 8.00 | 16.00 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | |
| 1.00 | 12.00 | 0.00 | 0.2889 | 0.2875 | 0.2875 | 0.2875 | 0.2875 | 0.2875 | |
| 1.00 | 12.00 | 4.00 | 0.2035 | 0.2026 | 0.2026 | 0.2026 | 0.2026 | 0.2026 | |
| 1.00 | 12.00 | 8.00 | 0.0566 | 0.0563 | 0.0563 | 0.0563 | 0.0563 | 0.0563 | |
| 1.00 | 12.00 | 12.00 | 0.0051 | 0.0051 | 0.0051 | 0.0051 | 0.0051 | 0.0051 | |
| 1.00 | 12.00 | 16.00 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | |
| 1.00 | 16.00 | 0.00 | 0.0796 | 0.0793 | 0.0793 | 0.0793 | 0.0793 | 0.0793 | |
| 1.00 | 16.00 | 4.00 | 0.0563 | 0.0561 | 0.0561 | 0.0561 | 0.0561 | 0.0561 | |
| 1.00 | 16.00 | 8.00 | 0.0162 | 0.0162 | 0.0162 | 0.0162 | 0.0162 | 0.0162 | |
| 1.00 | 16.00 | 12.00 | 0.0016 | 0.0016 | 0.0016 | 0.0016 | 0.0016 | 0.0016 | |
| 1.00 | 16.00 | 16.00 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | |
| 1.00 | 20.00 | 0.00 | 0.0124 | 0.0124 | 0.0124 | 0.0124 | 0.0124 | 0.0124 | |
| 1.00 | 20.00 | 4.00 | 0.0088 | 0.0088 | 0.0088 | 0.0088 | 0.0088 | 0.0088 | |
| 1.00 | 20.00 | 8.00 | 0.0027 | 0.0027 | 0.0027 | 0.0027 | 0.0027 | 0.0027 | |
| 1.00 | 20.00 | 12.00 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | |
| 1.00 | 20.00 | 16.00 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| 3.00 | 0.00 | 0.00 | 1.0847 | 0.8546 | 0.8580 | 0.8581 | 0.8581 | 0.8581 | |
| 3.00 | 0.00 | 4.00 | 0.7562 | 0.6017 | 0.6040 | 0.6040 | 0.6040 | 0.6040 | |
| 3.00 | 0.00 | 8.00 | 0.1925 | 0.1652 | 0.1659 | 0.1659 | 0.1659 | 0.1659 | |
| 3.00 | 0.00 | 12.00 | 0.0132 | 0.0146 | 0.0146 | 0.0146 | 0.0146 | 0.0146 | |
| 3.00 | 0.00 | 16.00 | 0.0003 | 0.0005 | 0.0005 | 0.0005 | 0.0005 | 0.0005 | |
| 3.00 | 4.00 | 0.00 | 1.0180 | 0.7991 | 0.8023 | 0.8023 | 0.8023 | 0.8023 | |
| 3.00 | 4.00 | 4.00 | 0.7096 | 0.5625 | 0.5646 | 0.5646 | 0.5646 | 0.5646 | |
| 3.00 | 4.00 | 8.00 | 0.1806 | 0.1542 | 0.1548 | 0.1548 | 0.1548 | 0.1548 | |
| 3.00 | 4.00 | 12.00 | 0.0124 | 0.0136 | 0.0136 | 0.0136 | 0.0136 | 0.0136 | |
| 3.00 | 4.00 | 16.00 | 0.0003 | 0.0004 | 0.0004 | 0.0004 | 0.0004 | 0.0004 | |
| 3.00 | 8.00 | 0.00 | 0.7539 | 0.5929 | 0.5951 | 0.5951 | 0.5951 | 0.5951 | |
| 3.00 | 8.00 | 4.00 | 0.5256 | 0.4173 | 0.4188 | 0.4188 | 0.4188 | 0.4188 | |
| 3.00 | 8.00 | 8.00 | 0.1338 | 0.1144 | 0.1148 | 0.1148 | 0.1148 | 0.1148 | |
| 3.00 | 8.00 | 12.00 | 0.0092 | 0.0101 | 0.0101 | 0.0101 | 0.0101 | 0.0101 | |
| 3.00 | 8.00 | 16.00 | 0.0002 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | |

Table 4. (Continued)

| t | y | z | Transient with NGC= 10 | 20 | 30 | 40 | 50 | 100 | Steady State |
|---|---|---|---|---|---|---|---|---|---|
| | | | ------------------ | ------------------ | C/C$_o$ | ------------------ | ------------------ | ------------------ | |
| 3.00 | 12.00 | 0.00 | 0.3534 | 0.2865 | 0.2877 | 0.2877 | 0.2877 | 0.2877 | |
| 3.00 | 12.00 | 4.00 | 0.2466 | 0.2020 | 0.2028 | 0.2028 | 0.2028 | 0.2028 | |
| 3.00 | 12.00 | 8.00 | 0.0632 | 0.0562 | 0.0564 | 0.0564 | 0.0564 | 0.0564 | |
| 3.00 | 12.00 | 12.00 | 0.0045 | 0.0051 | 0.0051 | 0.0051 | 0.0051 | 0.0051 | |
| 3.00 | 12.00 | 16.00 | 0.0001 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | |
| 3.00 | 16.00 | 0.00 | 0.0886 | 0.0791 | 0.0794 | 0.0794 | 0.0794 | 0.0794 | |
| 3.00 | 16.00 | 4.00 | 0.0620 | 0.0560 | 0.0562 | 0.0562 | 0.0562 | 0.0562 | |
| 3.00 | 16.00 | 8.00 | 0.0162 | 0.0162 | 0.0162 | 0.0162 | 0.0162 | 0.0162 | |
| 3.00 | 16.00 | 12.00 | 0.0013 | 0.0016 | 0.0016 | 0.0016 | 0.0016 | 0.0016 | |
| 3.00 | 16.00 | 16.00 | 0.0000 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | |
| 3.00 | 20.00 | 0.00 | 0.0113 | 0.0124 | 0.0124 | 0.0124 | 0.0124 | 0.0124 | |
| 3.00 | 20.00 | 4.00 | 0.0080 | 0.0088 | 0.0088 | 0.0088 | 0.0088 | 0.0088 | |
| 3.00 | 20.00 | 8.00 | 0.0022 | 0.0027 | 0.0027 | 0.0027 | 0.0027 | 0.0027 | |
| 3.00 | 20.00 | 12.00 | 0.0002 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | |
| 3.00 | 20.00 | 16.00 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| 5.00 | 0.00 | 0.00 | 0.2828 | 0.8266 | 0.8590 | 0.8580 | 0.8581 | 0.8581 | 0.8637 |
| 5.00 | 0.00 | 4.00 | 0.2054 | 0.5822 | 0.6046 | 0.6039 | 0.6040 | 0.6040 | 0.6061 |
| 5.00 | 0.00 | 8.00 | 0.0676 | 0.1590 | 0.1660 | 0.1659 | 0.1659 | 0.1659 | 0.1670 |
| 5.00 | 0.00 | 12.00 | 0.0098 | 0.0144 | 0.0146 | 0.0146 | 0.0146 | 0.0146 | 0.0131 |
| 5.00 | 0.00 | 16.00 | 0.0006 | 0.0005 | 0.0005 | 0.0005 | 0.0005 | 0.0005 | 0.0002 |
| 5.00 | 4.00 | 0.00 | 0.2627 | 0.7736 | 0.8032 | 0.8023 | 0.8023 | 0.8023 | 0.8058 |
| 5.00 | 4.00 | 4.00 | 0.1907 | 0.5448 | 0.5652 | 0.5646 | 0.5646 | 0.5646 | 0.5655 |
| 5.00 | 4.00 | 8.00 | 0.0625 | 0.1484 | 0.1549 | 0.1548 | 0.1548 | 0.1548 | 0.1558 |
| 5.00 | 4.00 | 12.00 | 0.0091 | 0.0133 | 0.0136 | 0.0136 | 0.0136 | 0.0136 | 0.0122 |
| 5.00 | 4.00 | 16.00 | 0.0005 | 0.0005 | 0.0004 | 0.0004 | 0.0004 | 0.0004 | 0.0002 |
| 5.00 | 8.00 | 0.00 | 0.1966 | 0.5744 | 0.5958 | 0.5951 | 0.5951 | 0.5951 | 0.5960 |
| 5.00 | 8.00 | 4.00 | 0.1427 | 0.4045 | 0.4193 | 0.4188 | 0.4188 | 0.4188 | 0.4183 |
| 5.00 | 8.00 | 8.00 | 0.0468 | 0.1102 | 0.1149 | 0.1148 | 0.1148 | 0.1148 | 0.1153 |
| 5.00 | 8.00 | 12.00 | 0.0068 | 0.0099 | 0.0101 | 0.0101 | 0.0101 | 0.0101 | 0.0090 |
| 5.00 | 8.00 | 16.00 | 0.0004 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0002 |
| 5.00 | 12.00 | 0.00 | 0.1024 | 0.2764 | 0.2879 | 0.2877 | 0.2877 | 0.2877 | 0.2901 |
| 5.00 | 12.00 | 4.00 | 0.0746 | 0.1950 | 0.2029 | 0.2028 | 0.2028 | 0.2028 | 0.2036 |
| 5.00 | 12.00 | 8.00 | 0.0252 | 0.0542 | 0.0564 | 0.0564 | 0.0564 | 0.0564 | 0.0561 |
| 5.00 | 12.00 | 12.00 | 0.0037 | 0.0051 | 0.0051 | 0.0051 | 0.0051 | 0.0051 | 0.0044 |
| 5.00 | 12.00 | 16.00 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0001 |
| 5.00 | 16.00 | 0.00 | 0.0352 | 0.0761 | 0.0794 | 0.0794 | 0.0794 | 0.0794 | 0.0796 |
| 5.00 | 16.00 | 4.00 | 0.0258 | 0.0539 | 0.0562 | 0.0562 | 0.0562 | 0.0562 | 0.0559 |
| 5.00 | 16.00 | 8.00 | 0.0091 | 0.0157 | 0.0162 | 0.0162 | 0.0162 | 0.0162 | 0.0154 |
| 5.00 | 16.00 | 12.00 | 0.0014 | 0.0016 | 0.0016 | 0.0016 | 0.0016 | 0.0016 | 0.0012 |
| 5.00 | 16.00 | 16.00 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0000 |
| 5.00 | 20.00 | 0.00 | 0.0082 | 0.0122 | 0.0124 | 0.0124 | 0.0124 | 0.0124 | 0.0112 |
| 5.00 | 20.00 | 4.00 | 0.0060 | 0.0087 | 0.0088 | 0.0088 | 0.0088 | 0.0088 | 0.0079 |
| 5.00 | 20.00 | 8.00 | 0.0022 | 0.0027 | 0.0027 | 0.0027 | 0.0027 | 0.0027 | 0.0022 |
| 5.00 | 20.00 | 12.00 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0002 |
| 5.00 | 20.00 | 16.00 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |

Table 5. Solute transport with $v=20$, $R=1$, $t_o=0.51$, $\mu=0$, $\lambda=0$, $D_x=10$, and $D_r=5$ according to scenario 4 at $x=10$ with $a=5$ for a third-type inlet condition calculated with the solution T4 of Table 1 using various values of NGC

| | | NGC= | | | | | |
|---|---|---|---|---|---|---|---|
| | | 10 | 25 | 50 | 100 | 200 | 400 |
| $t$ | $r$ | $C/C_o$ | | | | | |
| 0.50 | 0.00 | 0.4772 | 0.4750 | 0.4747 | 0.4746 | 0.4746 | 0.4746 |
| 0.50 | 2.00 | 0.4405 | 0.4382 | 0.4378 | 0.4378 | 0.4377 | 0.4377 |
| 0.50 | 4.00 | 0.3054 | 0.3032 | 0.3029 | 0.3028 | 0.3028 | 0.3028 |
| 0.50 | 6.00 | 0.1230 | 0.1217 | 0.1215 | 0.1215 | 0.1214 | 0.1214 |
| 0.50 | 8.00 | 0.0242 | 0.0238 | 0.0237 | 0.0237 | 0.0237 | 0.0237 |
| 0.50 | 10.00 | 0.0022 | 0.0022 | 0.0022 | 0.0022 | 0.0022 | 0.0022 |
| 1.00 | 0.00 | 0.4433 | 0.4456 | 0.4458 | 0.4459 | 0.4459 | 0.4459 |
| 1.00 | 2.00 | 0.4001 | 0.4020 | 0.4022 | 0.4022 | 0.4022 | 0.4022 |
| 1.00 | 4.00 | 0.2791 | 0.2800 | 0.2800 | 0.2800 | 0.2800 | 0.2800 |
| 1.00 | 6.00 | 0.1350 | 0.1351 | 0.1351 | 0.1351 | 0.1351 | 0.1351 |
| 1.00 | 8.00 | 0.0417 | 0.0415 | 0.0415 | 0.0415 | 0.0415 | 0.0415 |
| 1.00 | 10.00 | 0.0080 | 0.0079 | 0.0079 | 0.0079 | 0.0079 | 0.0079 |
| 1.50 | 0.00 | 0.0126 | 0.0084 | 0.0084 | 0.0084 | 0.0084 | 0.0084 |
| 1.50 | 2.00 | 0.0110 | 0.0076 | 0.0076 | 0.0076 | 0.0076 | 0.0076 |
| 1.50 | 4.00 | 0.0076 | 0.0056 | 0.0056 | 0.0056 | 0.0056 | 0.0056 |
| 1.50 | 6.00 | 0.0046 | 0.0032 | 0.0033 | 0.0033 | 0.0033 | 0.0033 |
| 1.50 | 8.00 | 0.0018 | 0.0015 | 0.0015 | 0.0015 | 0.0015 | 0.0015 |
| 1.50 | 10.00 | 0.0005 | 0.0005 | 0.0005 | 0.0005 | 0.0005 | 0.0005 |
| 2.00 | 0.00 | -0.0278 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0001 |
| 2.00 | 2.00 | -0.0245 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0001 |
| 2.00 | 4.00 | -0.0159 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 2.00 | 6.00 | -0.0073 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 2.00 | 8.00 | -0.0012 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 2.00 | 10.00 | 0.0001 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |

The third example concerns solute movement from a rectangular source at the soil surface. Table 4 contains $C(y,z,t)$ profiles calculated with the solution for scenario T2 in Table 1 using NGC=10, 20, 30, 40, 50, and 100 for $t=1$, 3, and 5; and $C(y,z)$ profiles calculated with the steady state solution SS2 in Table 1. In order to make a meaningful comparison between the two solutions, a relatively small value was selected for $D_x$ in the transient problem since the steady-state solution ignores longitudinal dispersion. Initially, the values for $C(y,z,t)$ calculated with NGC=10 or 20 are greater than the more accurate results obtained with NGC$\geq$30 as can be seen for $t=1$ or 3. For larger times (e.g., $t=5$), the solute profile approaches steady state and the use of a coarse grid for the numerical integration (NGC$\leq$20) leads to underestimation of the concentration. For NGC$\geq$30 the transient solution for t=5 closely resembles the simplified steady-state solution.

Our final example deals with a cylindrical geometry. Solutions for a cylindrical geometry require more computer time as compared to problems involving rectangular coordinates because of double integration. Table 5 contains $C(r,t)$ profiles at $x=10$ as a result of the application of a solute pulse, of duration 0.51, from a circular area at the soil surface. Because of the abrupt change in influent concentration at $t=0.51$, the use of a small NGC value will lead to poor predictions of the solute concentration. However, the calculated concentrations are quite similar for NGC>50. In all cases $C$ approaches zero for larger times, as mandated by the limited time during which the solute is applied.

From these and other examples it appears that a value of 100 is in most cases a reasonable selection for NGC. However, a higher value may be needed in some cases, such as for an abrupt change in concentration for small changes in the independent variable. The value for NGC needs to be specified in the input file (Appendix B). Numerical results for the three-dimensional solutions generally compared favorably with the simpler steady-state and one-dimensional solutions. It should be emphasized that the program is less suitable for predicting concentrations if $x$, $t$, $R$, $D_x$, $D_y$ or $D_r$, and $D_z$ approach zero. The program will generate solute concentrations for $t \approx 0$ based upon the initial condition and, sometimes, approximate the concentration at $x \approx 0$. The user should always provide input data that are physically and mathematically suitable for the analytical expressions in Table 1.

# 4. PROGRAM DESCRIPTION

The 3DADE code is written in Fortran. A complete listing of the program is provided in Appendix E. The main section of the code performs the following tasks:

(i) Reading the names of input and output files; default names can be specified in the main program. The program will not be executed if the input file does not exist. Note that no provisions are taken against overwriting existing output files.

(ii) Reading the input file and checking for apparent errors in the input data. The input file format is given in Appendix B. For the *direct* problem, the temporal and spatial grid system where the concentrations need to be calculated is read in (Appendix C1). For the *indirect* problem, the observed concentrations with corresponding time and location are read in (Appendix D1); the program uses the counter NOB to determine the total number of observations that are read in.

(iii) Initializing the problem by writing a heading of the output file and specifying the number of model parameters and independent variables in accordance with the selected model. For the *indirect* problem, the suitability of the specified fitting parameters is determined and the experimental data are written to the output file.

(iv) Executing the direct or indirect problem. In the *direct* problem, the coordinates $X(J=1,I)$ of the temporal and spatial grid system are calculated, based on user specifications. Subroutine MODELS, which calculates the concentration, is called each time a new grid coordinate is calculated. For the *indirect* problem, the subroutine MODELS is called for the whole observation set. The program then readjusts the model parameters to be fitted, according to a minimization of the sum of squares of the residuals between observed and newly predicted concentrations based on the maximum neighborhood method of *Marquardt* [1963]. This is done with the help of subroutine MATINV. The nonlinear least-squares inversion approach implemented in 3DADE was taken from *Parker and van Genuchten* [1984] with some changes and additions in the statistics regarding the goodness of the fit. The solution of the indirect problem is discussed in the next section.

(v) Writing results to the specified output file. For the *direct* problem the model parameters, concentrations and corresponding independent variables (i.e., $x$, $y$ or $r$, $z$, and $t$) are written to the output file. The following output is generated for the *indirect* problem: initial values for all model parameters; observed concentrations at specific times and locations; the sum of squares and values for the fitted parameters; the correlation matrix of the fitted model parameters; statistical information that can be used to assess the goodness of fit as discussed in the next section; and the observed and predicted concentrations (including their difference, i.e., the residual).

Three-dimensional problems may involve a large number of grid points or observed concentrations. The number of grid points can be reduced by utilizing symmetry in most physical problems as shown in Fig. 1; concentrations in certain regions of the solution domain can be deduced immediately from concentrations calculated in other regions. The program parameter NCON is used to define the size of several arrays for the indirect problem; NCON should be larger than the number of observed concentrations, although excessively large arrays should be avoided. If NCON is changed, the program needs to be recompiled prior to execution. NCON can be set to 1 for the solution of the direct or forward problem. During execution of the direct problem, the independent or dependent variables need not be stored in an array as they are written to the output file immediately after generation of the grid point and calculation of the concentration.

Subroutine MODELS is used to calculate the transient and steady-state solute concentrations for rectangular and cylindrical coordinate systems according to the solutions listed in Table 1. This routine returns individual concentrations for the direct problem, and an array of size NOB with predicted concentrations for the indirect problem. The program first checks if the calculations in MODELS can be bypassed, for example when the concentration is given directly by the initial or boundary profiles sketched in Fig. 1. Also, the production part of the solution is bypassed when $\lambda=0$. Furthermore, because $\lambda$ is uniform throughout the medium, the production part of the concentration is only evaluated for the direct problem if the independent variable $x$ or $t$ changes. In this case the logical variable PROD is set to true. The integrals in the solutions are evaluated in subroutine

CHEBY. For models 1, 2, 3, 4, 7, 8, 9, and 10 in Table 1, the appropriate external functions CF1, CT1, CF2, CT2, CF4, CT4, CF5, and CT5 are called, while the external functions LAM2 and LAM4 are used for the production part. A second integration routine, CHEBYONE, is called in case two integrals need to be evaluated. The function EXF($A$,$B$) is used to evaluate the product of the exponential function, exp($A$), and the complementary error function, erfc($B$), whereas function EXPBI0($X$,$Y$) determines the product of the exponential function, exp($X$), and the zeroth order modified Bessel function, $I_0(Y)$.

A list of the main program variables is given in Appendix A. An outline of the format of the input file is given in Appendix B. This input file can be prepared by the user with any text editor. Note that none of the analytical solutions in Table 1 will actually use all of the input parameters specified in Appendix B; however, a "dummy" value should still be provided for parameters that are not part of the solution to comply with the input format according to Appendix B. An exception is the indirect problem involving steady-state solutions (models 11, 12, and 13) for which no time of observation needs to be specified in the input file. As can be seen in Appendix B, the last part of the input file differs for the *direct* and *indirect* problems. The observed concentrations, as well as their location and time of observation, are specified in the input file using the free format for the indirect problem. The user can readily customize the input and output format of 3DADE, as needed. Appendices C and D deal with the forward (or direct) problem and contain data that were used to prepare some of the illustrations in *Leij et al.* [1991*b*]. Appendices C and D list the input file for five different examples, whereas Appendix D contains the corresponding output.

# 5. INDIRECT PROBLEM

## 5.1. *Parameter Optimization*

Program 3DADE allows model parameters to be estimated by fitting the analytical solutions from Table 1 to observed data. The parameter optimization routine was previously used by *van Genuchten* [1980, 1981] and *Parker and van Genuchten* [1984] to analyze experimentally determined solute concentration profiles. The program attempts to minimize the sum of squares of the residuals (i.e., the difference between the observed and the analytically predicted concentrations) by adjusting the model parameters that were marked as fitting parameters in the input file. Optimization is halted if the relative change in all fitted model parameters becomes less than STOPCR, whose value can be set in the source code, or if the maximum number of iterations (MIT) as specified in the input file, is exceeded. *Daniel and Wood* [1973] provide further theoretical background on the optimization technique.

Goodness of fit can be assessed in various ways, although it may be difficult to objectively characterize the correctness of these type of nonlinear optimizations. The value of $r^2$ for the regression of observed versus predicted (fitted) concentrations is calculated in the program with [*Myers*, 1986]:

$$r^2 = 1 - \frac{\sum_{i=1}^{N} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{N} (y_i - \bar{y})^2} \tag{8}$$

where $y_i$ and $\hat{y}_i$ are the observed and predicted dependent variables (concentrations) for the $i$th set of independent variables, and $\bar{y}$ is the mean of all $N$ observed concentrations. A value for $r^2$ close to unity indicates a good fit whereas low values are indicative of a poor description of the observed data by the selected analytical model. The mean-square error, *MSE*, is calculated according to

$$MSE = \frac{SSQ}{N-NP} \tag{9}$$

$$SSQ = \sum_{i=1}^{N} d_i^2 \qquad d_i = y_i - \hat{y}_i \tag{10}$$

where *NP* is the number of model parameters to be optimized, *SSQ* is the sum of squared differences in which $d_i$ is the difference between observed and predicted concentrations for the *i*th data pair. As can be seen, low values for MSE suggest a good fit. Partitioning of the sum of squares gives an estimate of the bias in the model and variability in the observations as follows:

$$SSQ = \sum_{i=1}^{N} d_i^2 = \underbrace{\bar{d}^2}_{\text{bias}} + \underbrace{\sum_{i=1}^{N} (d_i - \bar{d})^2}_{\text{variance}} \tag{11}$$

The program provides values for the bias and variance as a percentage of SSQ. For low values of SSQ, the (relative) value of the model bias gives relatively little information regarding the goodness of the fit. The output file of 3DADE also reports the mean, standard error, *T*-value, and the upper and lower limits of the 95% confidence interval for the model parameters after the final fit. The values for *T* and the standard error provide relative and absolute measures of deviations around the mean parameter values; a high value for *T* is desirable. Furthermore, one would like mean parameter values to be positioned in relatively narrow confidence intervals.

The parameters that can be fitted with 3DADE are $v$, $R$, $t_o$, $D_x$, $D_y$ or $D_r$, $D_z$, $\mu$, and $\lambda$. We have assumed that $C_o$, $a$, $b$, $x_1$, and $x_2$ are always known and need not be fitted; a unique solution of the indirect problem for unknown geometry parameters $a$, $b$, $x_1$, and $x_2$ will generally be difficult, although possible for some transport problems. Because formally the multidimensional analytical models are valid only for porous media that are uniform in all spatial directions with steady downward flow, it is to be expected that solutions of the indirect problem for such multidimensional problems will lead to results that may not be as reliable as those for one-dimensional displacement experiments (e.g., for laboratory columns). Moreover, few suitable field data sets were available on which the optimization procedure could be tested. Therefore, we relied in this report on generic data sets to illustrate the curve fitting part of 3DADE.

## 5.2. *Guidelines and Examples*

This section gives some general guidelines for the parameter optimization process and will then present four examples for which the inverse problem is solved. We found that it is generally best to have a large data set. On the other hand, the use of observations from a small spatial and temporal domain may lead to more uniform experimental conditions to which analytical models can be applied more successfully. In that case it is advantageous to restrict the number of observations to be fitted as much as possible. Because of potential nonuniqueness in the optimization problem, it is important that reliable initial estimates be provided. The fitting procedure, therefore, should be repeated for various combinations of initial estimates. One recommend scenario is to use for the first couple of optimizations a relatively large number of model parameters; parameters for which a reliable value is known from an independent source should be excluded. The number of fitting parameters for subsequent optimizations could be reduced based upon inspection of the correlation matrix: if there is a high correlation between two fitting parameters, one of these could be fixed at a constant value in a subsequent run of 3DADE. The minimum number of parameters to be fitted in 3DADE is two while no simultaneous fit of $v$ and $R$ is possible. The input file should contain a sufficient number of observations along the transverse coordinates to fit the transverse dispersion coefficients $D_y$, $D_z$, and $D_r$. In analogy to one-dimensional displacement experiments [*Parker and van Genuchten*, 1984], the concentration profile versus $x$ or $t$ needs to include data with sufficient resolution to warrant fitting of $v$ or $R$ and $D_x$.

Appendix E and F contains the input and output for four examples involving the indirect problem; note that the "observations" are based on the output of the direct problem. The first example considers solute application from the soil surface according to scenario 1 in Fig. 1. The concentrations were taken from a breakthrough curve, $C(t)$, calculated at $(x, y, z) = (20, -10, -10)$ and the steady transverse profile, $C(y)$, for $(x, z, t) = (20, -10, 2)$ generated with $\{v, R, t_o, \mu, \lambda, D_x, D_y, D_z\} = \{50, 1, 10, 0, 0, 20, 10, 5\}$. Using an initial estimate of $\{1, 10, 5\}$ for the fitting parameters $\{R, D_x, D_y\}$ the program obtained estimates which were fairly close to the actual values after three iterations. The second example

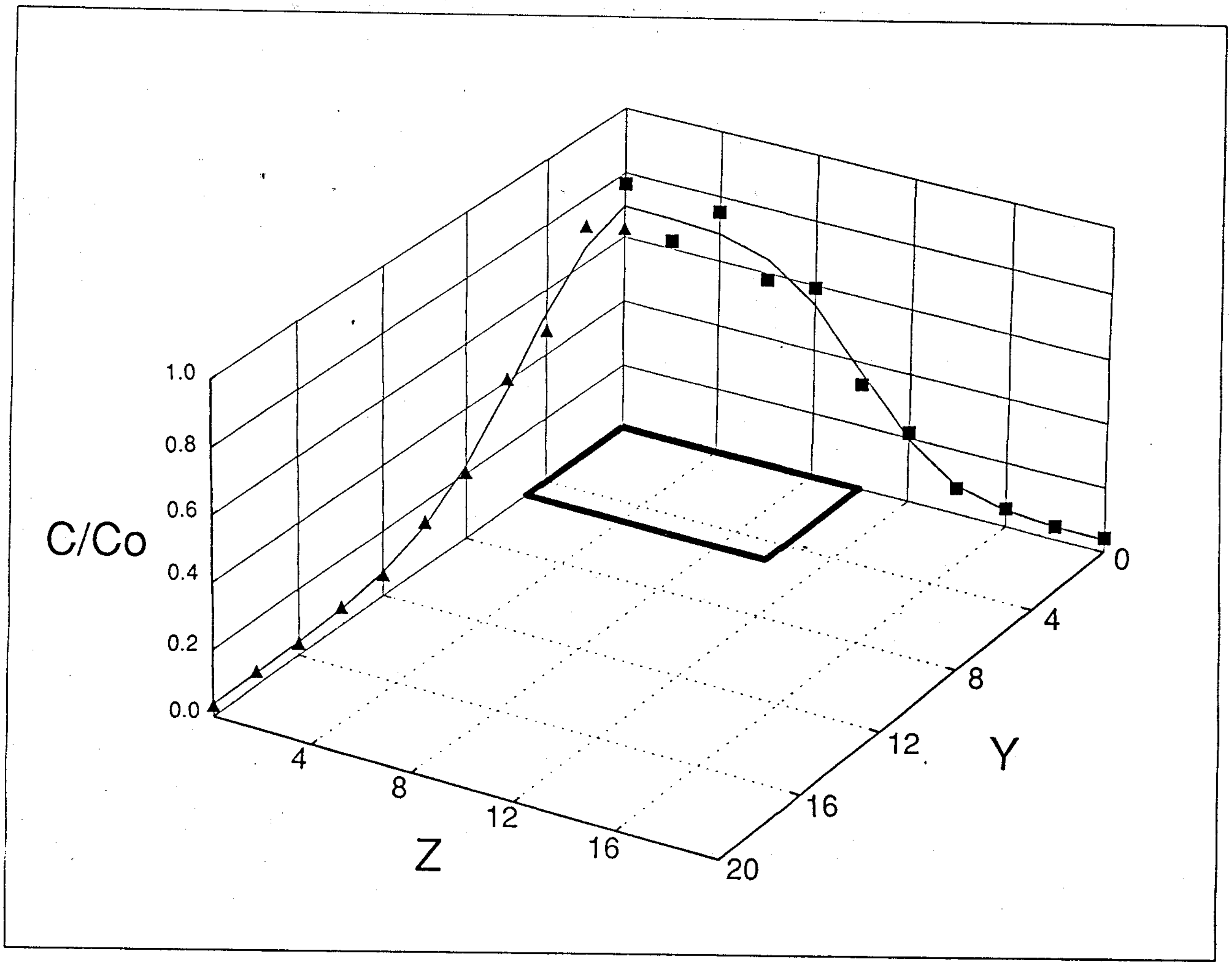



Fig. 2. Optimization of transverse solute distributions where the concentration values are 10 % below or above the value predicted with model 6. Solid lines denote fitted curves at $x=30$ and $t=2$ using the final parameters from example 3 in Appendix D2, while "observed" data points are represented as ▲ and ■.

involves the estimation of a relatively large parameter set from data generated with $\{v, R, \mu, \lambda, D_x, D_y, D_z\} = \{10, 2.5, 0.1, 0.05, 20, 10, 5\}$ for transport scenario 3 (Fig. 1). The observations consist of breakthrough curves at ten positions along the $x$ coordinate, and transverse profiles for $(x, z, t) = (30, 0, 2)$ and $(x, y, t) = (30, 0, 2)$. Using the initial set $\{R, \mu, \lambda, D_x, D_y, D_z\} = \{1, 0.01, 0.01, 50, 5, 2.5\}$, fitted model parameters were almost identical to the actual values after nine iterations. For this ideal example, a perfect correlation existed between "observed" and predicted concentrations whereas the fitted parameters were located in a very small confidence interval. Also note from the correlation matrix that the correlation between individual model parameters was generally small; this suggests that all six fitting parameters were needed to describe the data with the analytical model. This optimization example was repeated for a data set in which errors of $\pm 10$ % were imposed on the transverse concentration profiles of the previous example. Figure 2 shows the "observed" concentrations and the fitted curve at $x=30$ and $t=2$ along the two transverse $y$ and $z$ axes. The solute was initially present between depths 10 and 30, and in the transverse plane, as shown in Fig. 2 for $y<5$ and $z<10$. The analytical model could still describe the data reasonably well. Notice from the output that the MSE is nonzero, and that the lack of fit is completely due to the variability in the data.

Our final example 4 concerns the application of a solute pulse from a circular area at the soil surface. Due to the numerical integrations, this example will require a considerable amount of computer time, although the number of "observations" had been limited. The data consist of a longitudinal and a transverse profile at $t=0.5$ generated with $\{v, R, t_o, \mu, \lambda, D_x, D_r\} = \{20, 1, 0.25, 0, 0, 40, 10\}$. The program did reproduce the correct values for $\{t_o, D_x, D_r\}$ after five iteration steps using the initial parameter set $\{0.1, 20, 20\}$.

The 3DADE parameter optimization code produced excellent fits between observed and predicted concentrations for the examples discussed in this report. However, we stress again that for most practical cases one should not expect equally good results because of nonideal experimental conditions which likely will not meet the strict limitations imposed upon the problem by virtue of its analytical solution.

# 6. SUMMARY AND CONCLUSIONS

This report describes the 3DADE computer program for analytically modeling three-dimensional solute transport in homogeneous porous media as described with the advection-dispersion equation (including solute retardation, first-order decay, and zero-order production). The program augments the mathematical formulations and derivations by *Leij et al.* [1991*b*]. The code can be used to solve the direct problem for which concentrations are calculated as a function of time and space for specified model parameters, as well as the indirect problem for which the program estimates selected parameters by fitting an analytical solution to specified experimental data. Transient analytical solutions were evaluated for five different transport scenarios, i.e., three boundary-value problems and two initial-value problems. Simple steady-state solutions were also provided for the three boundary value problems. We emphasized that the utility of the analytical solutions in this report is somewhat restricted since actual experimental conditions deviate from the idealized conditions to which analytical solutions can be applied.

This report demonstrated the correctness of the solutions for some special cases where existing one-dimensional or steady-state solutions can be used. We also illustrated the sensitivity of the predicted concentrations to the number of Gauss-Chebyshev integration points used in the numerical integration routines of 3DADE. In general, 100 points in the Gauss-Chebyshev quadrature proved to be adequate for ensuring accurate integration.

The structure of the program and the tasks of the various sections of the code were briefly reviewed. The optimization of model parameter was discussed in somewhat greater detail using four fitting exercises. The program adequately estimated the model parameters for the four synthetic data sets. Appendices are provided that document the main program variables and the input file format. Listings of sample input and output files as well as the FORTRAN source code are also included.

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| *Variable* | *Description* |
|---|---|
| a | Name for variable C(2), i.e., dimension along *y*- or *r*-coordinate (Fig.1). |
| b | Name for variable C(3), i.e., dimension along the *z*-coordinate (Fig.1). |
| B(I) | Vector containing values for model parameters $v$, $R$, $t_o$, $\mu$, $\lambda$, $D_x$, $D_y$ or $D_r$, and $D_z$. In subroutine MODELS these parameters are redefined as V, R, TO, RMU, RLAM, DX, DY, and DZ. |
| BI(I) | Vector of names for parameters B(I) (specified as program parameters). |
| C(I) | Vector containing values for model constants $C_o$, $a$, $b$, $x_1$, and $x_2$, respectively. In subroutine MODELS these are redefined as CO, A, B, X1, and X2. |
| CN(I) | Vector of names for model constants C(I) (specified as program parameters). |
| Co | Name for variable C(1), i.e., (reference) concentration of inlet or initial distribution as sketched in Fig.1. |
| Dr | Name for variable B(7), i.e., dispersion coefficient in *r*-direction. |
| Dx | Name for variable B(6), i.e., dispersion coefficient in *x*-direction. |
| DX(I) | Increments in *t*, *x*, *y* or *r*, and *z*, respectively, used for specifying nodes for which the concentrations need to be calculated. |
| Dy | Name for variable B(7), i.e., dispersion coefficient in *y*-direction. |
| Dz | Name for variable B(8), i.e., dispersion coefficient in *z*-direction. |
| F(I) | Vector containing the fitted concentrations at X(J,I) after NIT iterations for the inverse problem. |
| IND | Variable to indicate if indirect (IND=1) or direct problem (IND=0) is to be solved. |
| INDEX(I) | Index for each model parameter. If INDEX(I)=0, the value specified for B(I) in the input file is assumed to be known and kept constant; if INDEX(I)=1, the coefficient is assumed to be unknown and fitted to the data. The value for INDEX is only relevant for NOB>0 and MIT>0. |
| LAM | Name for variable B(5), i.e., zero-order rate coefficient for production ($\lambda>0$). |
| MAXTRY | Maximum number of trials allowed within an iteration to find new parameter values that decrease SSQ (the value for MAXTRY is set in the program). |
| MIT | Maximum number of iterations allowed in the least-squares analysis. If MIT=0, the least-squares inversion part is bypassed and the program calculates and prints concentrations for given input values of *x*, *y* or *r*, *z*, and *t*, and using model parameters as specified in the input file; dummy variables of C(I) and INDEX(I), if specified, are still read but are not used in the program. |
| MODEL | Model number specifying the scenario and the type of inlet boundary condition. Model numbers 1 through 10 correspond to scenarios F1, T1, F2, T2, F3, T3, F4, T4, F5, and T5, respectively (cf. Fig. 1); a first-type condition is denoted with "F" and a third-type with "T". Models 11, 12, and 13 refer to the steady-state solutions for scenarios 1, 2, and 4, respectively. |
| MU | Name for variable B(4), i.e., first-order rate coefficient for decay ($\mu>0$) or accumulation ($\mu<0$). |

| *Variable* | *Description* |
|---|---|
| NCON | Array size to predict or fit concentrations (specified as a program parameter). |
| NGC | Number of intervals, *n*, in Gauss-Chebyshev quadrature. |
| NIT | Iteration number in least-squares analysis. |
| NIV | Number of independent variables, i.e., *x*, *y*, *z*, and *t* for models 1-6; *x*, *r*, and *t* for models 7-10; *x*, *y*, and *z* for models 11 and 12; and *x* and *r* for model 13. |
| NOB | Number of observations in the indirect problem; set to unity for the direct problem. Note that NOB cannot exceed NCON. |
| NP | Number of model parameters to be fitted to the observed data. |
| NUM | Number of nodal points for which concentration need to be calculated. |
| PROD | Logical variable for evaluating the production term. |
| PT | Adjusted time, $t$-$t_o$, for the concentration as a result of a pulse application. |
| R | Name for variable B(2), i.e., the retardation factor. |
| RHO | Dummy variable for integrals involving *r*. |
| STOPCR | Stop criterion. The curve fitting process stops when the relative change in the ratio of all coefficients becomes less than STOPCR (the value for STOPCR is specified in the program). |
| T | Time. |
| TAU | Dummy variable for integrals involving *t*. |
| TITLE | Character string to identify the transport problem. |
| To | Name for variable B(3), i.e., duration of solute application. |
| V | Name for variable B(1), i.e., pore-water velocity. |
| VN(I) | Vector of names for independent variables (specified as program parameters). |
| X | Distance along *x*-coordinate. |
| x1 | Name for variable C(4), i.e., depth along *x*-coordinate denoting the upper value of the initial solute distribution as sketched in Fig.1. |
| x2 | Name for variable C(5), i.e., depth along *x*-coordinate denoting the lower value of the initial solute distribution as sketched in Fig.1. |
| X(J,I) | Array which specifies the independent variables for each node as generated by the program using a specified step size, and the imposed lower and upper limits. J=1, 2, 3, and 4 refer to the *t*, *x*, *y* or *r*, and *z* coordinates, respectively, and I gives the node number. Hence, in order to predict the concentration at node I one has $t$=X(1,I), $x$=X(2,I), $y$ or $r$=X(3,I), and $z$=X(4,I). |
| XLOW(I) | Vector containing the lower limits for *t*, *x*, *y* or *r*, and *z*. For models 11-13 XLOW(1) is ignored. |
| XUP(I) | Vector containing the upper limits for *t*, *x*, *y* or *r*, and *z*. For scenarios 11-13 XUP(1) is ignored. |
| Y | Distance along *y*- or *r*-coordinate. |
| Y(I) | Vector containing the predicted concentrations at X(J,I) for the forward problem, and the observed concentrations for the inverse problem. |
| Z | Distance along *z*-coordinate. |

## APPENDIX B: INPUT FILE FORMAT

| *Line* | *Columns* | *Format* | *Variable* | *Comments* |
|---|---|---|---|---|
| 1 | | | | Dummy line to explain variables on next line. |
| 2 | 1-10 | I10 | MODEL | Model number. |
| | 11-20 | I10 | MIT | Maximum number of iterations. |
| | 21-30 | I10 | IND | Flag to indicate whether direct problem (IND=0) of indirect problem (IND=1) is to be solved. |
| | 31-40 | I10 | NGC | Number of intervals, i.e., $n$ in Eq. (7), in Gauss-Chebyshev quadrature. |
| 3 | 1-60 | A60 | TITLE | Comment to describe and identify problem and list dimensions. |
| 4 | | | | Dummy line to explain variables on next line. |
| 5 | 1-10 | F10.2 | B(9) | Value of $v$. |
| | 11-20 | F10.2 | B(10) | Value of $R$. |
| | 21-30 | F10.2 | B(11) | Value of $t_o$. |
| | 31-40 | F10.2 | B(12) | Value of $\mu$. |
| | 41-50 | F10.2 | B(13) | Value of $\lambda$. |
| 6 | 1-10 | I10 | INDEX(1) | Flag for fitting $v$ in indirect problem. |
| | 11-20 | I10 | INDEX(2) | Flag for fitting $R$ in indirect problem. |
| | 21-30 | I10 | INDEX(3) | Flag for fitting $t_o$ in indirect problem. |
| | 31-40 | I10 | INDEX(4) | Flag for fitting $\mu$ in indirect problem. |
| | 41-50 | I10 | INDEX(5) | Flag for fitting $\lambda$ in indirect problem. |
| 7 | | | | Dummy line to explain variables on next line. |
| 8 | 1-10 | F10.2 | B(14) | Value of $D_x$. |
| | 11-20 | F10.2 | B(15) | Value of $D_y$ or $D_r$. |
| | 21-30 | F10.2 | B(16) | Value of $D_z$. |
| 9 | 1-10 | I10 | INDEX(6) | Flag for fitting $D_x$ in indirect problem. |
| | 11-20 | I10 | INDEX(7) | Flag for fitting $D_y$ or $D_r$ in indirect problem. |
| | 21-30 | I10 | INDEX(8) | Flag for fitting $D_z$ in indirect problem. |
| 10 | | | | Dummy line to explain variables on next line. |
| 11 | 1-10 | F10.2 | C(1) | Value of $C_o$ |
| | 11-20 | F10.2 | C(2) | Value of $a$ |
| | 21-30 | F10.2 | C(3) | Value of $b$ |
| | 31-40 | F10.2 | C(4) | Value of $x_1$ |
| | 41-50 | F10.2 | C(5) | Value of $x_2$ |

| *Line* | *Columns* | *Format* | *Variable* | *Comments* |
|---|---|---|---|---|
| | | | **Direct Problem Only (NOB=0)** | |
| 12 | | | | Dummy line to explain variables on next line. |
| 13 | 1-10 | F10.2 | DX(1) | Increment in $t$. |
| | 11-20 | F10.2 | XLOW(1) | Lower limit of $t$. |
| | 21-30 | F10.2 | XUP(1) | Upper limit of $t$. |
| 14 | | | | Dummy line to explain variables on next line. |
| 15 | 1-10 | F10.2 | DX(2) | Increment in $x$. |
| | 11-20 | F10.2 | XLOW(2) | Lower limit of $x$. |
| | 21-30 | F10.2 | XUP(2) | Upper limit of $x$. |
| 16 | | | | Dummy line to explain variables on next line. |
| 17 | 1-10 | F10.2 | DX(3) | Increment in $y$ or $r$. |
| | 11-20 | F10.2 | XLOW(3) | Lower limit of $y$ or $r$. |
| | 21-30 | F10.2 | XUP(3) | Upper limit of $y$ or $r$. |
| 18 | | | | Dummy line to explain variables on next line. |
| 19 | 1-10 | F10.2 | DX(4) | Increment in $z$. |
| | 11-20 | F10.2 | XLOW(4) | Lower limit of $z$. |
| | 21-30 | F10.2 | XUP(4) | Upper limit of $z$. |
| | | | **Indirect Problem Only (NOB>0)** | |
| *For transient case* (MODEL≤10) | | | | |
| ≥12 | * | * | Y(I) | Value of $I$th observed concentration. |
| | * | * | X(1,I) | Value of $t$ for $I$th observation. |
| | * | * | X(2,1) | Value of $x$ for $I$th observation. |
| | * | * | X(3,I) | Value of $y$ or $r$ for $I$th observation. |
| | * | * | X(4,I) | Value of $z$, if applicable, for $I$th observation. |
| *For steady case* (MODEL>10) | | | | |
| ≥12 | * | * | X(2,1) | Value of $x$ for $I$th observation. |
| | * | * | X(3,I) | Value of $y$ or $r$ for $I$th observation. |
| | * | * | X(4,I) | Value of $z$, if applicable, for $I$th observation. |

The program will read data using the free format until the end of the file is encountered; no values for $z$ are needed for problems involving cylindrical coordinate systems.

# APPENDIX C: INPUT FILES FOR DIRECT PROBLEM

```
    model  max iter  indirect  #gaucheb
       11         0         0       100
EXAMPLE 1: FIGURE 2A
        v         R        to        mu    lambda
     50.0       1.0       0.0       0.0       0.0
        0         0         0         0         0
       Dx        Dy        Dz
     20.0      10.0      10.0
        0         0         0
       Co         a         b        x1        x2
      1.0       0.0       0.0       0.0       0.0
       dt      tmin      tmax
      0.0       0.0       0.0
       dx      xmin      xmax
     25.0       0.0      50.0
       dy      ymin      ymax
      5.0     -15.0      15.0
       dz      zmin      zmax
      0.0      -5.0       0.0

    model  max iter  indirect  #gaucheb
        3         0         0       100
EXAMPLE 2: FIGURE 4
        v         R        to        mu    lambda
     10.0       1.0    1000.0       0.0       0.0
        0         0         0         0         0
       Dx        Dy        Dz
    100.0      10.0      10.0
        0         0         0
       Co         a         b        x1        x2
      1.0       7.5       7.5       0.0       0.0
       dt      tmin      tmax
      0.0       1.0       1.0
       dx      xmin      xmax
     10.0       0.0      30.0
       dy      ymin      ymax
      5.0     -20.0      20.0
       dz      zmin      zmax
      0.0       0.0       0.0

    model  max iter  indirect  #gaucheb
        4         0         0       100
EXAMPLE 3: FIGURE 4
        v         R        to        mu    lambda
     10.0       1.0    1000.0       0.0       0.0
        0         0         0         0         0
       Dx        Dy        Dz
    100.0      10.0      10.0
        0         0         0
       Co         a         b        x1        x2
      1.0       7.5       7.5       0.0       0.0
       dt      tmin      tmax
      0.0       1.0       1.0
       dx      xmin      xmax
     10.0       0.0      30.0
       dy      ymin      ymax
      5.0     -20.0      20.0
       dz      zmin      zmax
      0.0       0.0       0.0
```

```
     model  max iter  indirect  #gaucheb
         6         0         0       100
EXAMPLE 4: FIGURE 3B
         v         R        to        mu    lambda
       0.0       1.5       0.0      0.25       0.5
         0         0         0         0         0
        Dx        Dy        Dz
     100.0      10.0      10.0
         0         0         0
        Co         a         b        x1        x2
       1.0       7.5       7.5       5.0      25.0
        dt      tmin      tmax
       0.0       1.0       1.0
        dx      xmin      xmax
       5.0       0.0     100.0
        dy      ymin      ymax
       0.0       0.0       0.0
        dz      zmin      zmax
       0.0       0.0       0.0

     model  max iter  indirect  #gaucheb
         8         0         0       100
EXAMPLE 5: FIGURE 7
         v         R        to        mu    lambda
      50.0       1.0       1.0       0.0       0.0
         0         0         0         0         0
        Dx        Dy        Dz
      20.0      10.0       0.0
         0         0         0
        Co         a         b        x1        x2
       1.0       7.5       0.0       0.0       0.0
        dt      tmin      tmax
       0.5       0.5       2.0
        dx      xmin      xmax
      25.0      25.0      50.0
        dy      ymin      ymax
       5.0       0.0      20.0
        dz      zmin      zmax
       0.0       0.0       0.0
```

## APPENDIX D: OUTPUT FILES FOR DIRECT PROBLEM

```
*******************************************************************
*                                                                 *
*                             3DADE                               *
*                                                                 *
*     ANALYTICAL SOLUTIONS FOR SOLUTE TRANSPORT IN 3-D SEMI-      *
*       INFINITE POROUS MEDIA (WRR 27(10):2719-2733, 1991)        *
*        WITH FITTING BY NONLINEAR LEAST SQUARES ANALYSIS         *
*                                                                 *
*                                                                 *
*     EXAMPLE 1: FIGURE 2A                                        *
*                                                                 *
*     MODEL 11                                   STEADY STATE     *
*     SCENARIO 1: SOLUTE APPLICATION FROM A SEMI-INFINITE         *
*                 QUADRANT OF AN INFINITE SOIL SURFACE            *
*                                                                 *
*******************************************************************
```

MODEL PARAMETERS

| NAME | VALUE |
|---|---|
| V | 50.00 |
| Dy | 10.00 |
| Dz | 10.00 |

CONSTANTS

| NAME | VALUE |
|---|---|
| Co | 1.00 |

INDEPENDENT VARIABLES

| VARIABLE | INCREMENT | MINIMUM | MAXIMUM |
|---|---|---|---|
| x | 25.000 | .000 | 50.000 |
| y | 5.000 | -15.000 | 15.000 |
| z | .000 | -5.000 | .000 |

PREDICTED CONCENTRATIONS

| NO | C | C/Co | x | y | z |
|---|---|---|---|---|---|
| 1 | 1.0000 | 1.0000 | .00 | -15.00 | -5.00 |
| 2 | 1.0000 | 1.0000 | .00 | -10.00 | -5.00 |
| 3 | 1.0000 | 1.0000 | .00 | -5.00 | -5.00 |
| 4 | .5000 | .5000 | .00 | .00 | -5.00 |
| 5 | .0000 | .0000 | .00 | 5.00 | -5.00 |
| 6 | .0000 | .0000 | .00 | 10.00 | -5.00 |
| 7 | .0000 | .0000 | .00 | 15.00 | -5.00 |
| 8 | .9431 | .9431 | 25.00 | -15.00 | -5.00 |
| 9 | .9423 | .9423 | 25.00 | -10.00 | -5.00 |
| 10 | .8894 | .8894 | 25.00 | -5.00 | -5.00 |
| 11 | .4715 | .4715 | 25.00 | .00 | -5.00 |
| 12 | .0537 | .0537 | 25.00 | 5.00 | -5.00 |
| 13 | .0007 | .0007 | 25.00 | 10.00 | -5.00 |
| 14 | .0000 | .0000 | 25.00 | 15.00 | -5.00 |
| 15 | .8679 | .8679 | 50.00 | -15.00 | -5.00 |
| 16 | .8572 | .8572 | 50.00 | -10.00 | -5.00 |
| 17 | .7538 | .7538 | 50.00 | -5.00 | -5.00 |
| 18 | .4341 | .4341 | 50.00 | .00 | -5.00 |
| 19 | .1144 | .1144 | 50.00 | 5.00 | -5.00 |
| 20 | .0110 | .0110 | 50.00 | 10.00 | -5.00 |
| 21 | .0003 | .0003 | 50.00 | 15.00 | -5.00 |

END OF PROBLEM

```
*******************************************************************
*                                                                 *
*                              3DADE                              *
*                                                                 *
*     ANALYTICAL SOLUTIONS FOR SOLUTE TRANSPORT IN 3-D SEMI-      *
*       INFINITE POROUS MEDIA (WRR 27(10):2719-2733, 1991)        *
*        WITH FITTING BY NONLINEAR LEAST SQUARES ANALYSIS         *
*                                                                 *
*                                                                 *
*     EXAMPLE 2: FIGURE 4                                         *
*                                                                 *
*     MODEL 3                        FIRST-TYPE INLET CONDITION   *
*     SCENARIO 2: SOLUTE APPLICATION FROM A RECTANGULAR           *
*                 SOURCE AT THE SOIL SURFACE                      *
*                                                                 *
*******************************************************************
```

MODEL PARAMETERS

| NAME | VALUE |
|---|---|
| V | 10.00 |
| R | 1.00 |
| To | 1000.00 |
| MU | .00 |
| LAM | .00 |
| Dx | 100.00 |
| Dy | 10.00 |
| Dz | 10.00 |

CONSTANTS

| NAME | VALUE |
|---|---|
| Co | 1.00 |
| a | 7.50 |
| b | 7.50 |

INDEPENDENT VARIABLES

| VARIABLE | INCREMENT | MINIMUM | MAXIMUM |
|---|---|---|---|
| t | .000 | 1.000 | 1.000 |
| x | 10.000 | .000 | 30.000 |
| y | 5.000 | -20.000 | 20.000 |
| z | .000 | .000 | .000 |

PREDICTED CONCENTRATIONS

| NO | C | C/Co | t | x | y | z |
|---|---|---|---|---|---|---|
| 1 | .0000 | .0000 | 1.00 | .00 | -20.00 | .00 |
| 2 | .0000 | .0000 | 1.00 | .00 | -15.00 | .00 |
| 3 | .0000 | .0000 | 1.00 | .00 | -10.00 | .00 |
| 4 | 1.0000 | 1.0000 | 1.00 | .00 | -5.00 | .00 |
| 5 | 1.0000 | 1.0000 | 1.00 | .00 | .00 | .00 |
| 6 | 1.0000 | 1.0000 | 1.00 | .00 | 5.00 | .00 |
| 7 | .0000 | .0000 | 1.00 | .00 | 10.00 | .00 |
| 8 | .0000 | .0000 | 1.00 | .00 | 15.00 | .00 |
| 9 | .0000 | .0000 | 1.00 | .00 | 20.00 | .00 |
| 10 | .0001 | .0001 | 1.00 | 10.00 | -20.00 | .00 |
| 11 | .0058 | .0058 | 1.00 | 10.00 | -15.00 | .00 |
| 12 | .1145 | .1145 | 1.00 | 10.00 | -10.00 | .00 |
| 13 | .5869 | .5869 | 1.00 | 10.00 | -5.00 | .00 |
| 14 | .6899 | .6899 | 1.00 | 10.00 | .00 | .00 |
| 15 | .5869 | .5869 | 1.00 | 10.00 | 5.00 | .00 |
| 16 | .1145 | .1145 | 1.00 | 10.00 | 10.00 | .00 |
| 17 | .0058 | .0058 | 1.00 | 10.00 | 15.00 | .00 |
| 18 | .0001 | .0001 | 1.00 | 10.00 | 20.00 | .00 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 19 | .0002 | .0002 | 1.00 | 20.00 | -20.00 | .00 |
| 20 | .0066 | .0066 | 1.00 | 20.00 | -15.00 | .00 |
| 21 | .0806 | .0806 | 1.00 | 20.00 | -10.00 | .00 |
| 22 | .2701 | .2701 | 1.00 | 20.00 | -5.00 | .00 |
| 23 | .3377 | .3377 | 1.00 | 20.00 | .00 | .00 |
| 24 | .2701 | .2701 | 1.00 | 20.00 | 5.00 | .00 |
| 25 | .0806 | .0806 | 1.00 | 20.00 | 10.00 | .00 |
| 26 | .0066 | .0066 | 1.00 | 20.00 | 15.00 | .00 |
| 27 | .0002 | .0002 | 1.00 | 20.00 | 20.00 | .00 |
| 28 | .0001 | .0001 | 1.00 | 30.00 | -20.00 | .00 |
| 29 | .0032 | .0032 | 1.00 | 30.00 | -15.00 | .00 |
| 30 | .0303 | .0303 | 1.00 | 30.00 | -10.00 | .00 |
| 31 | .0882 | .0882 | 1.00 | 30.00 | -5.00 | .00 |
| 32 | .1122 | .1122 | 1.00 | 30.00 | .00 | .00 |
| 33 | .0882 | .0882 | 1.00 | 30.00 | 5.00 | .00 |
| 34 | .0303 | .0303 | 1.00 | 30.00 | 10.00 | .00 |
| 35 | .0032 | .0032 | 1.00 | 30.00 | 15.00 | .00 |
| 36 | .0001 | .0001 | 1.00 | 30.00 | 20.00 | .00 |

END OF PROBLEM

```
****************************************************************
*                                                              *
*                           3DADE                              *
*                                                              *
*     ANALYTICAL SOLUTIONS FOR SOLUTE TRANSPORT IN 3-D SEMI-   *
*       INFINITE POROUS MEDIA (WRR 27(10):2719-2733, 1991)     *
*         WITH FITTING BY NONLINEAR LEAST SQUARES ANALYSIS     *
*                                                              *
*                                                              *
*     EXAMPLE 3: FIGURE 4                                      *
*                                                              *
*     MODEL 4                      THIRD-TYPE INLET CONDITION  *
*     SCENARIO 2: SOLUTE APPLICATION FROM A RECTANGULAR        *
*                 SOURCE AT THE SOIL SURFACE                   *
*                                                              *
****************************************************************
```

MODEL PARAMETERS

| NAME | VALUE |
|---|---|
| V | 10.00 |
| R | 1.00 |
| To | 1000.00 |
| MU | .00 |
| LAM | .00 |
| Dx | 100.00 |
| Dy | 10.00 |
| Dz | 10.00 |

CONSTANTS

| NAME | VALUE |
|---|---|
| Co | 1.00 |
| a | 7.50 |
| b | 7.50 |

INDEPENDENT VARIABLES

| VARIABLE | INCREMENT | MINIMUM | MAXIMUM |
|---|---|---|---|
| t | .000 | 1.000 | 1.000 |
| x | 10.000 | .000 | 30.000 |
| y | 5.000 | -20.000 | 20.000 |
| z | .000 | .000 | .000 |

PREDICTED CONCENTRATIONS

| NO | C | C/Co | t | x | y | z |
|---|---|---|---|---|---|---|
| 1 | .0001 | .0001 | 1.00 | .00 | -20.00 | .00 |
| 2 | .0037 | .0037 | 1.00 | .00 | -15.00 | .00 |
| 3 | .0695 | .0695 | 1.00 | .00 | -10.00 | .00 |
| 4 | .6428 | .6428 | 1.00 | .00 | -5.00 | .00 |
| 5 | .7051 | .7051 | 1.00 | .00 | .00 | .00 |
| 6 | .6428 | .6428 | 1.00 | .00 | 5.00 | .00 |
| 7 | .0695 | .0695 | 1.00 | .00 | 10.00 | .00 |
| 8 | .0037 | .0037 | 1.00 | .00 | 15.00 | .00 |
| 9 | .0001 | .0001 | 1.00 | .00 | 20.00 | .00 |
| 10 | .0002 | .0002 | 1.00 | 10.00 | -20.00 | .00 |
| 11 | .0057 | .0057 | 1.00 | 10.00 | -15.00 | .00 |
| 12 | .0824 | .0824 | 1.00 | 10.00 | -10.00 | .00 |
| 13 | .3282 | .3282 | 1.00 | 10.00 | -5.00 | .00 |
| 14 | .3994 | .3994 | 1.00 | 10.00 | .00 | .00 |
| 15 | .3282 | .3282 | 1.00 | 10.00 | 5.00 | .00 |
| 16 | .0824 | .0824 | 1.00 | 10.00 | 10.00 | .00 |
| 17 | .0057 | .0057 | 1.00 | 10.00 | 15.00 | .00 |
| 18 | .0002 | .0002 | 1.00 | 10.00 | 20.00 | .00 |
| 19 | .0001 | .0001 | 1.00 | 20.00 | -20.00 | .00 |
| 20 | .0039 | .0039 | 1.00 | 20.00 | -15.00 | .00 |
| 21 | .0412 | .0412 | 1.00 | 20.00 | -10.00 | .00 |
| 22 | .1287 | .1287 | 1.00 | 20.00 | -5.00 | .00 |
| 23 | .1622 | .1622 | 1.00 | 20.00 | .00 | .00 |
| 24 | .1287 | .1287 | 1.00 | 20.00 | 5.00 | .00 |
| 25 | .0412 | .0412 | 1.00 | 20.00 | 10.00 | .00 |
| 26 | .0039 | .0039 | 1.00 | 20.00 | 15.00 | .00 |
| 27 | .0001 | .0001 | 1.00 | 20.00 | 20.00 | .00 |
| 28 | .0001 | .0001 | 1.00 | 30.00 | -20.00 | .00 |
| 29 | .0014 | .0014 | 1.00 | 30.00 | -15.00 | .00 |
| 30 | .0126 | .0126 | 1.00 | 30.00 | -10.00 | .00 |
| 31 | .0356 | .0356 | 1.00 | 30.00 | -5.00 | .00 |
| 32 | .0454 | .0454 | 1.00 | 30.00 | .00 | .00 |
| 33 | .0356 | .0356 | 1.00 | 30.00 | 5.00 | .00 |
| 34 | .0126 | .0126 | 1.00 | 30.00 | 10.00 | .00 |
| 35 | .0014 | .0014 | 1.00 | 30.00 | 15.00 | .00 |
| 36 | .0001 | .0001 | 1.00 | 30.00 | 20.00 | .00 |

END OF PROBLEM

```
*********************************************************************
*                                                                   *
*                             3DADE                                 *
*                                                                   *
*     ANALYTICAL SOLUTIONS FOR SOLUTE TRANSPORT IN 3-D SEMI-        *
*      INFINITE POROUS MEDIA (WRR 27(10):2719-2733, 1991)           *
*        WITH FITTING BY NONLINEAR LEAST SQUARES ANALYSIS           *
*                                                                   *
*                                                                   *
*     EXAMPLE 4: FIGURE 3B                                          *
*                                                                   *
*     MODEL 6                        THIRD-TYPE INLET CONDITION     *
*     SCENARIO 3: SOLUTE INITIALLY UNIFORMLY DISTRIBUTED IN A       *
*                 PARALLELEPIPEDAL REGION OF THE SOIL               *
*                                                                   *
*********************************************************************
```

MODEL PARAMETERS

| NAME | VALUE |
|---|---|
| V | .00 |
| R | 1.50 |
| MU | .25 |
| LAM | .50 |
| Dx | 100.00 |
| Dy | 10.00 |
| Dz | 10.00 |

CONSTANTS

| NAME | VALUE |
|---|---|
| Co | 1.00 |
| a | 7.50 |
| b | 7.50 |
| x1 | 5.00 |
| x2 | 25.00 |

INDEPENDENT VARIABLES

| VARIABLE | INCREMENT | MINIMUM | MAXIMUM |
|---|---|---|---|
| t | .000 | 1.000 | 1.000 |
| x | 5.000 | .000 | 100.000 |
| y | .000 | .000 | .000 |
| z | .000 | .000 | .000 |

PREDICTED CONCENTRATIONS

| NO | C | C/Co | t | x | y | z |
|---|---|---|---|---|---|---|
| 1 | .8022 | .8022 | 1.00 | .00 | .00 | .00 |
| 2 | .8117 | .8117 | 1.00 | 5.00 | .00 | .00 |
| 3 | .8268 | .8268 | 1.00 | 10.00 | .00 | .00 |
| 4 | .8180 | .8180 | 1.00 | 15.00 | .00 | .00 |
| 5 | .7640 | .7640 | 1.00 | 20.00 | .00 | .00 |
| 6 | .6683 | .6683 | 1.00 | 25.00 | .00 | .00 |
| 7 | .5555 | .5555 | 1.00 | 30.00 | .00 | .00 |
| 8 | .4544 | .4544 | 1.00 | 35.00 | .00 | .00 |
| 9 | .3818 | .3818 | 1.00 | 40.00 | .00 | .00 |
| 10 | .3393 | .3393 | 1.00 | 45.00 | .00 | .00 |
| 11 | .3189 | .3189 | 1.00 | 50.00 | .00 | .00 |
| 12 | .3107 | .3107 | 1.00 | 55.00 | .00 | .00 |
| 13 | .3080 | .3080 | 1.00 | 60.00 | .00 | .00 |
| 14 | .3073 | .3073 | 1.00 | 65.00 | .00 | .00 |
| 15 | .3071 | .3071 | 1.00 | 70.00 | .00 | .00 |
| 16 | .3071 | .3071 | 1.00 | 75.00 | .00 | .00 |
| 17 | .3070 | .3070 | 1.00 | 80.00 | .00 | .00 |
| 18 | .3070 | .3070 | 1.00 | 85.00 | .00 | .00 |
| 19 | .3070 | .3070 | 1.00 | 90.00 | .00 | .00 |
| 20 | .3070 | .3070 | 1.00 | 95.00 | .00 | .00 |
| 21 | .3070 | .3070 | 1.00 | 100.00 | .00 | .00 |

END OF PROBLEM

```
*********************************************************************
*                                                                   *
*                             3DADE                                 *
*                                                                   *
*     ANALYTICAL SOLUTIONS FOR SOLUTE TRANSPORT IN 3-D SEMI-        *
*       INFINITE POROUS MEDIA (WRR 27(10):2719-2733, 1991)          *
*        WITH FITTING BY NONLINEAR LEAST SQUARES ANALYSIS           *
*                                                                   *
*                                                                   *
*     EXAMPLE 5: FIGURE 7                                           *
*                                                                   *
*     MODEL 8                       THIRD-TYPE INLET CONDITION      *
*     SCENARIO 4: SOLUTE APPLICATION FROM A CIRCULAR                *
*                 SOURCE AT THE SOIL SURFACE                        *
*                                                                   *
*********************************************************************
```

MODEL PARAMETERS

| NAME | VALUE |
|---|---|
| V | 50.00 |
| R | 1.00 |
| To | 1.00 |
| MU | .00 |
| LAM | .00 |
| Dx | 20.00 |
| Dr | 10.00 |

CONSTANTS

| NAME | VALUE |
|---|---|
| Co | 1.00 |
| a | 7.50 |

INDEPENDENT VARIABLES

| VARIABLE | INCREMENT | MINIMUM | MAXIMUM |
|---|---|---|---|
| t | .500 | .500 | 2.000 |
| x | 25.000 | 25.000 | 50.000 |
| r | 5.000 | .000 | 20.000 |

PREDICTED CONCENTRATIONS

| NO | C | C/Co | t | x | r |
|---|---|---|---|---|---|
| 1 | .4791 | .4791 | .50 | 25.00 | .00 |
| 2 | .3623 | .3623 | .50 | 25.00 | 5.00 |
| 3 | .0766 | .0766 | .50 | 25.00 | 10.00 |
| 4 | .0019 | .0019 | .50 | 25.00 | 15.00 |
| 5 | .0000 | .0000 | .50 | 25.00 | 20.00 |
| 6 | .0000 | .0000 | .50 | 50.00 | .00 |
| 7 | .0000 | .0000 | .50 | 50.00 | 5.00 |
| 8 | .0000 | .0000 | .50 | 50.00 | 10.00 |
| 9 | .0000 | .0000 | .50 | 50.00 | 15.00 |
| 10 | .0000 | .0000 | .50 | 50.00 | 20.00 |
| 11 | .9352 | .9352 | 1.00 | 25.00 | .00 |
| 12 | .6984 | .6984 | 1.00 | 25.00 | 5.00 |
| 13 | .1636 | .1636 | 1.00 | 25.00 | 10.00 |
| 14 | .0065 | .0065 | 1.00 | 25.00 | 15.00 |
| 15 | .0000 | .0000 | 1.00 | 25.00 | 20.00 |
| 16 | .3940 | .3940 | 1.00 | 50.00 | .00 |
| 17 | .2905 | .2905 | 1.00 | 50.00 | 5.00 |

| | | | | | |
|---|---|---|---|---|---|
| 18 | .0995 | .0995 | 1.00 | 50.00 | 10.00 |
| 19 | .0124 | .0124 | 1.00 | 50.00 | 15.00 |
| 20 | .0005 | .0005 | 1.00 | 50.00 | 20.00 |
| 21 | .4561 | .4561 | 1.50 | 25.00 | .00 |
| 22 | .3361 | .3361 | 1.50 | 25.00 | 5.00 |
| 23 | .0871 | .0871 | 1.50 | 25.00 | 10.00 |
| 24 | .0046 | .0046 | 1.50 | 25.00 | 15.00 |
| 25 | .0000 | .0000 | 1.50 | 25.00 | 20.00 |
| 26 | .7535 | .7535 | 1.50 | 50.00 | .00 |
| 27 | .5596 | .5596 | 1.50 | 50.00 | 5.00 |
| 28 | .2024 | .2024 | 1.50 | 50.00 | 10.00 |
| 29 | .0295 | .0295 | 1.50 | 50.00 | 15.00 |
| 30 | .0016 | .0016 | 1.50 | 50.00 | 20.00 |
| 31 | .0000 | .0000 | 2.00 | 25.00 | .00 |
| 32 | .0000 | .0000 | 2.00 | 25.00 | 5.00 |
| 33 | .0000 | .0000 | 2.00 | 25.00 | 10.00 |
| 34 | .0000 | .0000 | 2.00 | 25.00 | 15.00 |
| 35 | .0000 | .0000 | 2.00 | 25.00 | 20.00 |
| 36 | .3598 | .3598 | 2.00 | 50.00 | .00 |
| 37 | .2694 | .2694 | 2.00 | 50.00 | 5.00 |
| 38 | .1031 | .1031 | 2.00 | 50.00 | 10.00 |
| 39 | .0172 | .0172 | 2.00 | 50.00 | 15.00 |
| 40 | .0011 | .0011 | 2.00 | 50.00 | 20.00 |

**END OF PROBLEM**

# APPENDIX E: INPUT FILES FOR INDIRECT PROBLEM

```
C
          1          20          1         100
1: TRANSIENT LONGITUDINAL AND STEADY TRANSVERSE PROFILE
C
       50.0         1.5      10.00         0.0         0.0
          0           1          0           0           0
C
       10.0         5.0        5.0
          1           1          0
C
        1.0         0.0        0.0         0.0         0.0
0.0000  0.10  20.00  -10.00 -10.00
0.0003  0.20  20.00  -10.00 -10.00
0.0883  0.30  20.00  -10.00 -10.00
0.5395  0.40  20.00  -10.00 -10.00
0.8889  0.50  20.00  -10.00 -10.00
0.9836  0.60  20.00  -10.00 -10.00
0.9977  0.70  20.00  -10.00 -10.00
0.9992  0.80  20.00  -10.00 -10.00
0.9993  0.90  20.00  -10.00 -10.00
0.9993  1.00  20.00  -10.00 -10.00
0.9993  2.00  20.00  -10.00 -10.00
0.9986  2.00  20.00  -9.00  -10.00
0.9968  2.00  20.00  -8.00  -10.00
0.9923  2.00  20.00  -7.00  -10.00
0.9821  2.00  20.00  -6.00  -10.00
0.9610  2.00  20.00  -5.00  -10.00
0.9220  2.00  20.00  -4.00  -10.00
0.8575  2.00  20.00  -3.00  -10.00
0.7627  2.00  20.00  -2.00  -10.00
0.6398  2.00  20.00  -1.00  -10.00
0.4998  2.00  20.00  0.00   -10.00
0.3598  2.00  20.00  1.00   -10.00
0.2370  2.00  20.00  2.00   -10.00
0.1422  2.00  20.00  3.00   -10.00
0.0776  2.00  20.00  4.00   -10.00
0.0386  2.00  20.00  5.00   -10.00
0.0176  2.00  20.00  6.00   -10.00
0.0073  2.00  20.00  7.00   -10.00
0.0028  2.00  20.00  8.00   -10.00
0.0010  2.00  20.00  9.00   -10.00
0.0003  2.00  20.00  10.00   -10.00

C
          6          20          1         100
2. TRANSIENT LONGITUDINAL AND TRANSVERSAL PROFILES
C
       10.0         1.0       0.00        0.01        0.01
          0           1          0           1           1
C
       50.0         5.0        2.5
          1           1          1
C
        1.0         5.0       10.0        10.0        30.0
     0.0161        0.50       5.00        0.00        0.00
     0.2420        0.50      10.00        0.00        0.00
     0.8381        0.50      15.00        0.00        0.00
     0.9757        0.50      20.00        0.00        0.00
     0.9715        0.50      25.00        0.00        0.00
     0.7458        0.50      30.00        0.00        0.00
     0.1497        0.50      35.00        0.00        0.00
     0.0122        0.50      40.00        0.00        0.00
     0.0099        0.50      45.00        0.00        0.00
```

```
     0.0099      0.50      50.00      0.00      0.00
     0.0280      1.00       5.00      0.00      0.00
     0.1601      1.00      10.00      0.00      0.00
     0.5505      1.00      15.00      0.00      0.00
     0.8469      1.00      20.00      0.00      0.00
     0.8928      1.00      25.00      0.00      0.00
     0.7656      1.00      30.00      0.00      0.00
     0.3754      1.00      35.00      0.00      0.00
     0.0788      1.00      40.00      0.00      0.00
     0.0222      1.00      45.00      0.00      0.00
     0.0196      1.00      50.00      0.00      0.00
     0.0322      1.50       5.00      0.00      0.00
     0.1163      1.50      10.00      0.00      0.00
     0.3649      1.50      15.00      0.00      0.00
     0.6642      1.50      20.00      0.00      0.00
     0.7942      1.50      25.00      0.00      0.00
     0.7405      1.50      30.00      0.00      0.00
     0.4946      1.50      35.00      0.00      0.00
     0.1951      1.50      40.00      0.00      0.00
     0.0556      1.50      45.00      0.00      0.00
     0.0308      1.50      50.00      0.00      0.00
     0.0336      2.00       5.00      0.00      0.00
     0.0921      2.00      10.00      0.00      0.00
     0.2546      2.00      15.00      0.00      0.00
     0.5023      2.00      20.00      0.00      0.00
     0.6798      2.00      25.00      0.00      0.00
     0.6966      2.00      30.00      0.00      0.00
     0.5484      2.00      35.00      0.00      0.00
     0.3017      2.00      40.00      0.00      0.00
     0.1170      2.00      45.00      0.00      0.00
     0.0508      2.00      50.00      0.00      0.00
     0.6966      2.00      30.00      0.00      0.00
     0.6504      2.00      30.00      2.00      0.00
     0.5279      2.00      30.00      4.00      0.00
     0.3708      2.00      30.00      6.00      0.00
     0.2271      2.00      30.00      8.00      0.00
     0.1265      2.00      30.00     10.00      0.00
     0.0719      2.00      30.00     12.00      0.00
     0.0486      2.00      30.00     14.00      0.00
     0.0409      2.00      30.00     16.00      0.00
     0.0389      2.00      30.00     18.00      0.00
     0.0385      2.00      30.00     20.00      0.00
     0.6966      2.00      30.00      0.00      0.00
     0.6954      2.00      30.00      0.00      2.00
     0.6857      2.00      30.00      0.00      4.00
     0.6451      2.00      30.00      0.00      6.00
     0.5390      2.00      30.00      0.00      8.00
     0.3677      2.00      30.00      0.00     10.00
     0.1963      2.00      30.00      0.00     12.00
     0.0902      2.00      30.00      0.00     14.00
     0.0496      2.00      30.00      0.00     16.00
     0.0400      2.00      30.00      0.00     18.00
     0.0386      2.00      30.00      0.00     20.00
C
          6        20          1       100
3: EXAMPLE 2 WITH MODIFIED TRANSVERSE PROFILES
C
       10.0       1.0       0.00      0.01      0.01
          0         1          0         1         1
C
       50.0       5.0        2.5
          1         1          1
C
        1.0       5.0       10.0      10.0      30.0
```

| | | | | |
|---|---|---|---|---|
| 0.0161 | 0.50 | 5.00 | 0.00 | 0.00 |
| 0.2420 | 0.50 | 10.00 | 0.00 | 0.00 |
| 0.8381 | 0.50 | 15.00 | 0.00 | 0.00 |
| 0.9757 | 0.50 | 20.00 | 0.00 | 0.00 |
| 0.9715 | 0.50 | 25.00 | 0.00 | 0.00 |
| 0.7458 | 0.50 | 30.00 | 0.00 | 0.00 |
| 0.1497 | 0.50 | 35.00 | 0.00 | 0.00 |
| 0.0122 | 0.50 | 40.00 | 0.00 | 0.00 |
| 0.0099 | 0.50 | 45.00 | 0.00 | 0.00 |
| 0.0099 | 0.50 | 50.00 | 0.00 | 0.00 |
| 0.0280 | 1.00 | 5.00 | 0.00 | 0.00 |
| 0.1601 | 1.00 | 10.00 | 0.00 | 0.00 |
| 0.5505 | 1.00 | 15.00 | 0.00 | 0.00 |
| 0.8469 | 1.00 | 20.00 | 0.00 | 0.00 |
| 0.8928 | 1.00 | 25.00 | 0.00 | 0.00 |
| 0.7656 | 1.00 | 30.00 | 0.00 | 0.00 |
| 0.3754 | 1.00 | 35.00 | 0.00 | 0.00 |
| 0.0788 | 1.00 | 40.00 | 0.00 | 0.00 |
| 0.0222 | 1.00 | 45.00 | 0.00 | 0.00 |
| 0.0196 | 1.00 | 50.00 | 0.00 | 0.00 |
| 0.0322 | 1.50 | 5.00 | 0.00 | 0.00 |
| 0.1163 | 1.50 | 10.00 | 0.00 | 0.00 |
| 0.3649 | 1.50 | 15.00 | 0.00 | 0.00 |
| 0.6642 | 1.50 | 20.00 | 0.00 | 0.00 |
| 0.7942 | 1.50 | 25.00 | 0.00 | 0.00 |
| 0.7405 | 1.50 | 30.00 | 0.00 | 0.00 |
| 0.4946 | 1.50 | 35.00 | 0.00 | 0.00 |
| 0.1951 | 1.50 | 40.00 | 0.00 | 0.00 |
| 0.0556 | 1.50 | 45.00 | 0.00 | 0.00 |
| 0.0308 | 1.50 | 50.00 | 0.00 | 0.00 |
| 0.0336 | 2.00 | 5.00 | 0.00 | 0.00 |
| 0.0921 | 2.00 | 10.00 | 0.00 | 0.00 |
| 0.2546 | 2.00 | 15.00 | 0.00 | 0.00 |
| 0.5023 | 2.00 | 20.00 | 0.00 | 0.00 |
| 0.6798 | 2.00 | 25.00 | 0.00 | 0.00 |
| 0.6966 | 2.00 | 30.00 | 0.00 | 0.00 |
| 0.5484 | 2.00 | 35.00 | 0.00 | 0.00 |
| 0.3017 | 2.00 | 40.00 | 0.00 | 0.00 |
| 0.1170 | 2.00 | 45.00 | 0.00 | 0.00 |
| 0.0508 | 2.00 | 50.00 | 0.00 | 0.00 |
| 0.6269 | 2.00 | 30.00 | 0.00 | 0.00 |
| 0.7154 | 2.00 | 30.00 | 2.00 | 0.00 |
| 0.4751 | 2.00 | 30.00 | 4.00 | 0.00 |
| 0.4078 | 2.00 | 30.00 | 6.00 | 0.00 |
| 0.2044 | 2.00 | 30.00 | 8.00 | 0.00 |
| 0.1392 | 2.00 | 30.00 | 10.00 | 0.00 |
| 0.0647 | 2.00 | 30.00 | 12.00 | 0.00 |
| 0.0535 | 2.00 | 30.00 | 14.00 | 0.00 |
| 0.0368 | 2.00 | 30.00 | 16.00 | 0.00 |
| 0.0428 | 2.00 | 30.00 | 18.00 | 0.00 |
| 0.0347 | 2.00 | 30.00 | 20.00 | 0.00 |
| 0.7663 | 2.00 | 30.00 | 0.00 | 0.00 |
| 0.6259 | 2.00 | 30.00 | 0.00 | 2.00 |
| 0.7543 | 2.00 | 30.00 | 0.00 | 4.00 |
| 0.5806 | 2.00 | 30.00 | 0.00 | 6.00 |
| 0.5929 | 2.00 | 30.00 | 0.00 | 8.00 |
| 0.3309 | 2.00 | 30.00 | 0.00 | 10.00 |
| 0.2159 | 2.00 | 30.00 | 0.00 | 12.00 |
| 0.0812 | 2.00 | 30.00 | 0.00 | 14.00 |
| 0.0546 | 2.00 | 30.00 | 0.00 | 16.00 |
| 0.0396 | 2.00 | 30.00 | 0.00 | 18.00 |
| 0.0425 | 2.00 | 30.00 | 0.00 | 20.00 |

```
C
         7        30         1       500
4: LONGITUDINAL AND TRANSVERSE PROFILE
C
      20.0       1.0      0.10       0.0       0.0
         0         0         1         0         0
C
      20.0      20.0       0.0
         1         1         1
C
       1.0       5.0       0.0       0.0       0.0
    0.0563      0.50      2.00      0.00
    0.1476      0.50      4.00      0.00
    0.2499      0.50      6.00      0.00
    0.3262      0.50      8.00      0.00
    0.3489      0.50     10.00      0.00
    0.3164      0.50     12.00      0.00
    0.2492      0.50     14.00      0.00
    0.1736      0.50     16.00      0.00
    0.1085      0.50     18.00      0.00
    0.0614      0.50     20.00      0.00
    0.3402      0.50     10.00      1.00
    0.3144      0.50     10.00      2.00
    0.2733      0.50     10.00      3.00
    0.2212      0.50     10.00      4.00
    0.1648      0.50     10.00      5.00
    0.1120      0.50     10.00      6.00
    0.0690      0.50     10.00      7.00
    0.0384      0.50     10.00      8.00
    0.0193      0.50     10.00      9.00
    0.0088      0.50     10.00     10.00
```

## APPENDIX F: OUTPUT FILES FOR INDIRECT PROBLEM

```
*******************************************************************
*                                                                 *
*                             3DADE                               *
*                                                                 *
*      ANALYTICAL SOLUTIONS FOR SOLUTE TRANSPORT IN 3-D SEMI-     *
*        INFINITE POROUS MEDIA (WRR 27(10):2719-2733, 1991)       *
*         WITH FITTING BY NONLINEAR LEAST SQUARES ANALYSIS        *
*                                                                 *
*     1: TRANSIENT LONGITUDINAL AND STEADY TRANSVERSE PROFILE     *
*                                                                 *
*     MODEL 1                          FIRST-TYPE INLET CONDITION *
*     SCENARIO 1: SOLUTE APPLICATION FROM A SEMI-INFINITE         *
*                 QUADRANT OF AN INFINITE SOIL SURFACE            *
*                                                                 *
*******************************************************************
```

INITIAL ESTIMATES OF MODEL PARAMETERS

| NAME | VALUE | FITTING |
|---|---|---|
| V | 50.00 | - |
| R | 1.50 | + |
| To | 10.00 | - |
| MU | .00 | - |
| LAM | .00 | - |
| Dx | 10.00 | + |
| Dy | 5.00 | + |
| Dz | 5.00 | - |

CONSTANTS

| NAME | VALUE |
|---|---|
| Co | 1.00 |

OBSERVED CONCENTRATIONS

| NO | C | t | x | y | z |
|---|---|---|---|---|---|
| 1 | .0000 | .1000 | 20.00 | -10.00 | -10.00 |
| 2 | .0003 | .2000 | 20.00 | -10.00 | -10.00 |
| 3 | .0883 | .3000 | 20.00 | -10.00 | -10.00 |
| 4 | .5395 | .4000 | 20.00 | -10.00 | -10.00 |
| 5 | .8889 | .5000 | 20.00 | -10.00 | -10.00 |
| 6 | .9836 | .6000 | 20.00 | -10.00 | -10.00 |
| 7 | .9977 | .7000 | 20.00 | -10.00 | -10.00 |
| 8 | .9992 | .8000 | 20.00 | -10.00 | -10.00 |
| 9 | .9993 | .9000 | 20.00 | -10.00 | -10.00 |
| 10 | .9993 | 1.0000 | 20.00 | -10.00 | -10.00 |
| 11 | .9993 | 2.0000 | 20.00 | -10.00 | -10.00 |
| 12 | .9986 | 2.0000 | 20.00 | -9.00 | -10.00 |
| 13 | .9968 | 2.0000 | 20.00 | -8.00 | -10.00 |
| 14 | .9923 | 2.0000 | 20.00 | -7.00 | -10.00 |
| 15 | .9821 | 2.0000 | 20.00 | -6.00 | -10.00 |
| 16 | .9610 | 2.0000 | 20.00 | -5.00 | -10.00 |
| 17 | .9220 | 2.0000 | 20.00 | -4.00 | -10.00 |
| 18 | .8575 | 2.0000 | 20.00 | -3.00 | -10.00 |
| 19 | .7627 | 2.0000 | 20.00 | -2.00 | -10.00 |
| 20 | .6398 | 2.0000 | 20.00 | -1.00 | -10.00 |
| 21 | .4998 | 2.0000 | 20.00 | .00 | -10.00 |
| 22 | .3598 | 2.0000 | 20.00 | 1.00 | -10.00 |
| 23 | .2370 | 2.0000 | 20.00 | 2.00 | -10.00 |
| 24 | .1422 | 2.0000 | 20.00 | 3.00 | -10.00 |
| 25 | .0776 | 2.0000 | 20.00 | 4.00 | -10.00 |
| 26 | .0386 | 2.0000 | 20.00 | 5.00 | -10.00 |
| 27 | .0176 | 2.0000 | 20.00 | 6.00 | -10.00 |
| 28 | .0073 | 2.0000 | 20.00 | 7.00 | -10.00 |
| 29 | .0028 | 2.0000 | 20.00 | 8.00 | -10.00 |
| 30 | .0010 | 2.0000 | 20.00 | 9.00 | -10.00 |
| 31 | .0003 | 2.0000 | 20.00 | 10.00 | -10.00 |

RESULTS FOR EACH ITERATION STEP

| STEP | SSQ | R | Dx | Dy |
|---|---|---|---|---|
| 0 | 1.16275 | 1.500 | 10.000 | 5.000 |
| 1 | .16941 | 1.204 | 41.242 | 8.713 |
| 2 | .01937 | .981 | 40.396 | 10.080 |
| 3 | .00204 | 1.001 | 14.845 | 9.982 |
| 4 | .00001 | 1.000 | 19.655 | 10.012 |
| 5 | .00000 | 1.000 | 20.023 | 10.014 |
| 6 | .00000 | 1.000 | 20.029 | 10.014 |

CORRELATION MATRIX

| | R | Dx | Dy |
|---|---|---|---|
| R | 1.0000 | | |
| Dx | .0854 | 1.0000 | |
| Dy | -.0011 | .0239 | 1.0000 |

r^2 FOR REGRESSION OF OBSERVED VS. PREDICTED VALUES = 1.000000

MEAN SQUARE FOR ERROR (MSE) = .000000

BIAS (%) = 64.14 VARIANCE (%) = 35.86

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

| VAR | NAME | VALUE | S.E.COEFF. | T-VALUE | 95% CONFIDENCE LIMITS LOWER | UPPER |
|---|---|---|---|---|---|---|
| 1 | R | 1.00005 | .0001 | 10085.93 | 1.000 | 1.000 |
| 2 | Dx | 20.02916 | .0290 | 690.32 | 19.970 | 20.089 |
| 3 | Dy | 10.01380 | .0075 | 1335.64 | 9.998 | 10.029 |

| ----ORDERED BY COMPUTER INPUT----- | | | | --------ORDERED BY RESIDUALS------ | | | |
|---|---|---|---|---|---|---|---|
| | CONCENTRATION | | RESI- | | CONCENTRATION | | RESI- |
| NO | OBS | FITTED | DUAL | NO | OBS | FITTED | DUAL |
| 1 | .000 | .000 | .000 | 4 | .540 | .539 | .000 |
| 2 | .000 | .000 | .000 | 2 | .000 | .000 | .000 |
| 3 | .088 | .088 | .000 | 5 | .889 | .889 | .000 |
| 4 | .540 | .539 | .000 | 1 | .000 | .000 | .000 |
| 5 | .889 | .889 | .000 | 30 | .001 | .001 | .000 |
| 6 | .984 | .984 | .000 | 27 | .018 | .018 | .000 |
| 7 | .998 | .998 | .000 | 31 | .000 | .000 | .000 |
| 8 | .999 | 1.000 | .000 | 29 | .003 | .003 | .000 |
| 9 | .999 | 1.000 | .000 | 28 | .007 | .007 | .000 |
| 10 | .999 | 1.000 | .000 | 19 | .763 | .763 | .000 |
| 11 | .999 | 1.000 | .000 | 18 | .858 | .858 | .000 |
| 12 | .999 | .999 | .000 | 3 | .088 | .088 | .000 |
| 13 | .997 | .997 | .000 | 26 | .039 | .039 | .000 |
| 14 | .992 | .993 | .000 | 20 | .640 | .640 | .000 |
| 15 | .982 | .982 | .000 | 17 | .922 | .922 | .000 |
| 16 | .961 | .961 | .000 | 21 | .500 | .500 | .000 |
| 17 | .922 | .922 | .000 | 25 | .078 | .078 | .000 |
| 18 | .858 | .858 | .000 | 24 | .142 | .142 | .000 |
| 19 | .763 | .763 | .000 | 23 | .237 | .237 | .000 |
| 20 | .640 | .640 | .000 | 6 | .984 | .984 | .000 |
| 21 | .500 | .500 | .000 | 22 | .360 | .360 | .000 |
| 22 | .360 | .360 | .000 | 16 | .961 | .961 | .000 |
| 23 | .237 | .237 | .000 | 15 | .982 | .982 | .000 |
| 24 | .142 | .142 | .000 | 8 | .999 | 1.000 | .000 |
| 25 | .078 | .078 | .000 | 14 | .992 | .993 | .000 |
| 26 | .039 | .039 | .000 | 7 | .998 | .998 | .000 |
| 27 | .018 | .018 | .000 | 9 | .999 | 1.000 | .000 |
| 28 | .007 | .007 | .000 | 13 | .997 | .997 | .000 |
| 29 | .003 | .003 | .000 | 10 | .999 | 1.000 | .000 |
| 30 | .001 | .001 | .000 | 11 | .999 | 1.000 | .000 |
| 31 | .000 | .000 | .000 | 12 | .999 | .999 | .000 |

END OF PROBLEM

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*****************************************************************
*                                                               *
*                            3DADE                              *
*                                                               *
*     ANALYTICAL SOLUTIONS FOR SOLUTE TRANSPORT IN 3-D SEMI-    *
*       INFINITE POROUS MEDIA (WRR 27(10):2719-2733, 1991)      *
*        WITH FITTING BY NONLINEAR LEAST SQUARES ANALYSIS       *
*                                                               *
*                                                               *
*    2. TRANSIENT LONGITUDINAL AND TRANSVERSAL PROFILES         *
*                                                               *
*    MODEL 6                      THIRD-TYPE INLET CONDITION    *
*    SCENARIO 3: SOLUTE INITIALLY UNIFORMLY DISTRIBUTED IN A    *
*                PARALLELEPIPEDAL REGION OF THE SOIL            *
*                                                               *
*****************************************************************
```

INITIAL ESTIMATES OF MODEL PARAMETERS

| NAME | VALUE | FITTING |
|---|---|---|
| V | 10.00 | - |
| R | 1.00 | + |
| MU | .01 | + |
| LAM | .01 | + |
| Dx | 50.00 | + |
| Dy | 5.00 | + |
| Dz | 2.50 | + |

CONSTANTS

| NAME | VALUE |
|---|---|
| Co | 1.00 |
| a | 5.00 |
| b | 10.00 |
| x1 | 10.00 |
| x2 | 30.00 |

OBSERVED CONCENTRATIONS

| NO | C | t | x | y | z |
|---|---|---|---|---|---|
| 1 | .0161 | .5000 | 5.00 | .00 | .00 |
| 2 | .2420 | .5000 | 10.00 | .00 | .00 |
| 3 | .8381 | .5000 | 15.00 | .00 | .00 |
| 4 | .9757 | .5000 | 20.00 | .00 | .00 |
| 5 | .9715 | .5000 | 25.00 | .00 | .00 |
| 6 | .7458 | .5000 | 30.00 | .00 | .00 |
| 7 | .1497 | .5000 | 35.00 | .00 | .00 |
| 8 | .0122 | .5000 | 40.00 | .00 | .00 |
| 9 | .0099 | .5000 | 45.00 | .00 | .00 |
| 10 | .0099 | .5000 | 50.00 | .00 | .00 |
| 11 | .0280 | 1.0000 | 5.00 | .00 | .00 |
| 12 | .1601 | 1.0000 | 10.00 | .00 | .00 |
| 13 | .5505 | 1.0000 | 15.00 | .00 | .00 |
| 14 | .8469 | 1.0000 | 20.00 | .00 | .00 |
| 15 | .8928 | 1.0000 | 25.00 | .00 | .00 |
| 16 | .7656 | 1.0000 | 30.00 | .00 | .00 |
| 17 | .3754 | 1.0000 | 35.00 | .00 | .00 |
| 18 | .0788 | 1.0000 | 40.00 | .00 | .00 |
| 19 | .0222 | 1.0000 | 45.00 | .00 | .00 |
| 20 | .0196 | 1.0000 | 50.00 | .00 | .00 |
| 21 | .0322 | 1.5000 | 5.00 | .00 | .00 |
| 22 | .1163 | 1.5000 | 10.00 | .00 | .00 |
| 23 | .3649 | 1.5000 | 15.00 | .00 | .00 |
| 24 | .6642 | 1.5000 | 20.00 | .00 | .00 |
| 25 | .7942 | 1.5000 | 25.00 | .00 | .00 |

| | | | | | |
|---|---|---|---|---|---|
| 26 | .7405 | 1.5000 | 30.00 | .00 | .00 |
| 27 | .4946 | 1.5000 | 35.00 | .00 | .00 |
| 28 | .1951 | 1.5000 | 40.00 | .00 | .00 |
| 29 | .0556 | 1.5000 | 45.00 | .00 | .00 |
| 30 | .0308 | 1.5000 | 50.00 | .00 | .00 |
| 31 | .0336 | 2.0000 | 5.00 | .00 | .00 |
| 32 | .0921 | 2.0000 | 10.00 | .00 | .00 |
| 33 | .2546 | 2.0000 | 15.00 | .00 | .00 |
| 34 | .5023 | 2.0000 | 20.00 | .00 | .00 |
| 35 | .6798 | 2.0000 | 25.00 | .00 | .00 |
| 36 | .6966 | 2.0000 | 30.00 | .00 | .00 |
| 37 | .5484 | 2.0000 | 35.00 | .00 | .00 |
| 38 | .3017 | 2.0000 | 40.00 | .00 | .00 |
| 39 | .1170 | 2.0000 | 45.00 | .00 | .00 |
| 40 | .0508 | 2.0000 | 50.00 | .00 | .00 |
| 41 | .6966 | 2.0000 | 30.00 | .00 | .00 |
| 42 | .6504 | 2.0000 | 30.00 | 2.00 | .00 |
| 43 | .5279 | 2.0000 | 30.00 | 4.00 | .00 |
| 44 | .3708 | 2.0000 | 30.00 | 6.00 | .00 |
| 45 | .2271 | 2.0000 | 30.00 | 8.00 | .00 |
| 46 | .1265 | 2.0000 | 30.00 | 10.00 | .00 |
| 47 | .0719 | 2.0000 | 30.00 | 12.00 | .00 |
| 48 | .0486 | 2.0000 | 30.00 | 14.00 | .00 |
| 49 | .0409 | 2.0000 | 30.00 | 16.00 | .00 |
| 50 | .0389 | 2.0000 | 30.00 | 18.00 | .00 |
| 51 | .0385 | 2.0000 | 30.00 | 20.00 | .00 |
| 52 | .6966 | 2.0000 | 30.00 | .00 | .00 |
| 53 | .6954 | 2.0000 | 30.00 | .00 | 2.00 |
| 54 | .6857 | 2.0000 | 30.00 | .00 | 4.00 |
| 55 | .6451 | 2.0000 | 30.00 | .00 | 6.00 |
| 56 | .5390 | 2.0000 | 30.00 | .00 | 8.00 |
| 57 | .3677 | 2.0000 | 30.00 | .00 | 10.00 |
| 58 | .1963 | 2.0000 | 30.00 | .00 | 12.00 |
| 59 | .0902 | 2.0000 | 30.00 | .00 | 14.00 |
| 60 | .0496 | 2.0000 | 30.00 | .00 | 16.00 |
| 61 | .0400 | 2.0000 | 30.00 | .00 | 18.00 |
| 62 | .0386 | 2.0000 | 30.00 | .00 | 20.00 |

RESULTS FOR EACH ITERATION STEP

| STEP | SSQ | R | MU | LAM | Dx | Dy | Dz |
|---|---|---|---|---|---|---|---|
| 0 | 3.37083 | 1.000 | .010 | .010 | 50.000 | 5.000 | 2.500 |
| 1 | 1.15105 | 2.078 | .122 | .034 | 66.550 | 9.649 | 2.137 |
| 2 | .40237 | 2.690 | .241 | .072 | 2.131 | 10.419 | 4.147 |
| 3 | .11132 | 2.570 | .424 | .113 | 6.333 | 7.657 | 3.862 |
| 4 | .01438 | 2.520 | .245 | .075 | 13.872 | 9.081 | 4.635 |
| 5 | .00026 | 2.501 | .122 | .053 | 19.069 | 9.835 | 4.926 |
| 6 | .00000 | 2.500 | .101 | .050 | 19.964 | 9.989 | 4.989 |
| 7 | .00000 | 2.500 | .100 | .050 | 19.997 | 9.999 | 4.999 |
| 8 | .00000 | 2.500 | .100 | .050 | 19.999 | 10.000 | 5.001 |
| 9 | .00000 | 2.500 | .100 | .050 | 19.999 | 10.000 | 5.001 |

CORRELATION MATRIX

| | R | MU | LAM | Dx | Dy | Dz |
|---|---|---|---|---|---|---|
| R | 1.0000 | | | | | |
| MU | .0122 | 1.0000 | | | | |
| LAM | .1289 | .7415 | 1.0000 | | | |
| Dx | .2004 | -.5506 | -.4643 | 1.0000 | | |
| Dy | .2007 | -.8408 | -.4094 | .2601 | 1.0000 | |
| Dz | -.0621 | .2421 | .2896 | -.1277 | -.0964 | 1.0000 |

r^2 FOR REGRESSION OF OBSERVED VS. PREDICTED VALUES = 1.000000

MEAN SQUARE FOR ERROR (MSE) = .000000

BIAS (%) = .02 VARIANCE (%) = 99.98

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

| VAR | NAME | VALUE | S.E.COEFF. | T-VALUE | 95% CONFIDENCE LIMITS LOWER | UPPER |
|---|---|---|---|---|---|---|
| 1 | R | 2.50009 | .0001 | 46341.00 | 2.500 | 2.500 |
| 2 | MU | .09999 | .0001 | 1675.88 | .100 | .100 |
| 3 | LAM | .04998 | .0000 | 4440.32 | .050 | .050 |
| 4 | Dx | 19.99930 | .0017 | 11498.64 | 19.996 | 20.003 |
| 5 | Dy | 10.00044 | .0012 | 8222.59 | 9.998 | 10.003 |
| 6 | Dz | 5.00096 | .0000 | 6559964.22 | 5.001 | 5.001 |

----ORDERED BY COMPUTER INPUT----- --------ORDERED BY RESIDUALS------

| NO | CONCENTRATION OBS | FITTED | RESIDUAL | NO | CONCENTRATION OBS | FITTED | RESIDUAL |
|---|---|---|---|---|---|---|---|
| 1 | .016 | .016 | .000 | 53 | .695 | .695 | .000 |
| 2 | .242 | .242 | .000 | 4 | .976 | .976 | .000 |
| 3 | .838 | .838 | .000 | 47 | .072 | .072 | .000 |
| 4 | .976 | .976 | .000 | 26 | .741 | .740 | .000 |
| 5 | .972 | .971 | .000 | 40 | .051 | .051 | .000 |
| 6 | .746 | .746 | .000 | 8 | .012 | .012 | .000 |
| 7 | .150 | .150 | .000 | 25 | .794 | .794 | .000 |
| 8 | .012 | .012 | .000 | 62 | .039 | .039 | .000 |
| 9 | .010 | .010 | .000 | 57 | .368 | .368 | .000 |
| 10 | .010 | .010 | .000 | 61 | .040 | .040 | .000 |
| 11 | .028 | .028 | .000 | 43 | .528 | .528 | .000 |
| 12 | .160 | .160 | .000 | 5 | .972 | .971 | .000 |
| 13 | .551 | .550 | .000 | 11 | .028 | .028 | .000 |
| 14 | .847 | .847 | .000 | 45 | .227 | .227 | .000 |
| 15 | .893 | .893 | .000 | 24 | .664 | .664 | .000 |
| 16 | .766 | .766 | .000 | 14 | .847 | .847 | .000 |
| 17 | .375 | .375 | .000 | 32 | .092 | .092 | .000 |
| 18 | .079 | .079 | .000 | 2 | .242 | .242 | .000 |
| 19 | .022 | .022 | .000 | 28 | .195 | .195 | .000 |
| 20 | .020 | .020 | .000 | 39 | .117 | .117 | .000 |
| 21 | .032 | .032 | .000 | 7 | .150 | .150 | .000 |
| 22 | .116 | .116 | .000 | 13 | .551 | .550 | .000 |
| 23 | .365 | .365 | .000 | 34 | .502 | .502 | .000 |
| 24 | .664 | .664 | .000 | 37 | .548 | .548 | .000 |
| 25 | .794 | .794 | .000 | 60 | .050 | .050 | .000 |
| 26 | .741 | .740 | .000 | 35 | .680 | .680 | .000 |
| 27 | .495 | .495 | .000 | 31 | .034 | .034 | .000 |
| 28 | .195 | .195 | .000 | 1 | .016 | .016 | .000 |
| 29 | .056 | .056 | .000 | 10 | .010 | .010 | .000 |
| 30 | .031 | .031 | .000 | 55 | .645 | .645 | .000 |
| 31 | .034 | .034 | .000 | 21 | .032 | .032 | .000 |
| 32 | .092 | .092 | .000 | 9 | .010 | .010 | .000 |
| 33 | .255 | .255 | .000 | 51 | .039 | .039 | .000 |
| 34 | .502 | .502 | .000 | 16 | .766 | .766 | .000 |
| 35 | .680 | .680 | .000 | 12 | .160 | .160 | .000 |
| 36 | .697 | .697 | .000 | 42 | .650 | .650 | .000 |
| 37 | .548 | .548 | .000 | 58 | .196 | .196 | .000 |
| 38 | .302 | .302 | .000 | 38 | .302 | .302 | .000 |
| 39 | .117 | .117 | .000 | 50 | .039 | .039 | .000 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 40 | .051 | .051 | .000 | 49 | .041 | .041 | .000 |
| 41 | .697 | .697 | .000 | 17 | .375 | .375 | .000 |
| 42 | .650 | .650 | .000 | 27 | .495 | .495 | .000 |
| 43 | .528 | .528 | .000 | 30 | .031 | .031 | .000 |
| 44 | .371 | .371 | .000 | 56 | .539 | .539 | .000 |
| 45 | .227 | .227 | .000 | 46 | .127 | .127 | .000 |
| 46 | .127 | .127 | .000 | 20 | .020 | .020 | .000 |
| 47 | .072 | .072 | .000 | 18 | .079 | .079 | .000 |
| 48 | .049 | .049 | .000 | 59 | .090 | .090 | .000 |
| 49 | .041 | .041 | .000 | 29 | .056 | .056 | .000 |
| 50 | .039 | .039 | .000 | 36 | .697 | .697 | .000 |
| 51 | .039 | .039 | .000 | 41 | .697 | .697 | .000 |
| 52 | .697 | .697 | .000 | 52 | .697 | .697 | .000 |
| 53 | .695 | .695 | .000 | 48 | .049 | .049 | .000 |
| 54 | .686 | .686 | .000 | 22 | .116 | .116 | .000 |
| 55 | .645 | .645 | .000 | 54 | .686 | .686 | .000 |
| 56 | .539 | .539 | .000 | 3 | .838 | .838 | .000 |
| 57 | .368 | .368 | .000 | 15 | .893 | .893 | .000 |
| 58 | .196 | .196 | .000 | 23 | .365 | .365 | .000 |
| 59 | .090 | .090 | .000 | 44 | .371 | .371 | .000 |
| 60 | .050 | .050 | .000 | 19 | .022 | .022 | .000 |
| 61 | .040 | .040 | .000 | 6 | .746 | .746 | .000 |
| 62 | .039 | .039 | .000 | 33 | .255 | .255 | .000 |

END OF PROBLEM

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*********************************************************************
*                                                                   *
*                              3DADE                                *
*                                                                   *
*     ANALYTICAL SOLUTIONS FOR SOLUTE TRANSPORT IN 3-D SEMI-        *
*       INFINITE POROUS MEDIA (WRR 27(10):2719-2733, 1991)          *
*        WITH FITTING BY NONLINEAR LEAST SQUARES ANALYSIS           *
*                                                                   *
*                                                                   *
*     3: EXAMPLE 2 WITH MODIFIED TRANSVERSE PROFILES                *
*                                                                   *
*     MODEL 6                        THIRD-TYPE INLET CONDITION     *
*     SCENARIO 3: SOLUTE INITIALLY UNIFORMLY DISTRIBUTED IN A       *
*                 PARALLELEPIPEDAL REGION OF THE SOIL               *
*                                                                   *
*********************************************************************
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INITIAL ESTIMATES OF MODEL PARAMETERS

| NAME | VALUE | FITTING |
|---|---|---|
| V | 10.00 | - |
| R | 1.00 | + |
| MU | .01 | + |
| LAM | .01 | + |
| Dx | 50.00 | + |
| Dy | 5.00 | + |
| Dz | 2.50 | + |

CONSTANTS

| NAME | VALUE |
|---|---|
| Co | 1.00 |
| a | 5.00 |
| b | 10.00 |
| x1 | 10.00 |
| x2 | 30.00 |

OBSERVED CONCENTRATIONS

| NO | C | t | x | y | z |
|---|---|---|---|---|---|
| 1 | .0161 | .5000 | 5.00 | .00 | .00 |
| 2 | .2420 | .5000 | 10.00 | .00 | .00 |
| 3 | .8381 | .5000 | 15.00 | .00 | .00 |
| 4 | .9757 | .5000 | 20.00 | .00 | .00 |
| 5 | .9715 | .5000 | 25.00 | .00 | .00 |
| 6 | .7458 | .5000 | 30.00 | .00 | .00 |
| 7 | .1497 | .5000 | 35.00 | .00 | .00 |
| 8 | .0122 | .5000 | 40.00 | .00 | .00 |
| 9 | .0099 | .5000 | 45.00 | .00 | .00 |
| 10 | .0099 | .5000 | 50.00 | .00 | .00 |
| 11 | .0280 | 1.0000 | 5.00 | .00 | .00 |
| 12 | .1601 | 1.0000 | 10.00 | .00 | .00 |
| 13 | .5505 | 1.0000 | 15.00 | .00 | .00 |
| 14 | .8469 | 1.0000 | 20.00 | .00 | .00 |
| 15 | .8928 | 1.0000 | 25.00 | .00 | .00 |
| 16 | .7656 | 1.0000 | 30.00 | .00 | .00 |
| 17 | .3754 | 1.0000 | 35.00 | .00 | .00 |
| 18 | .0788 | 1.0000 | 40.00 | .00 | .00 |
| 19 | .0222 | 1.0000 | 45.00 | .00 | .00 |
| 20 | .0196 | 1.0000 | 50.00 | .00 | .00 |
| 21 | .0322 | 1.5000 | 5.00 | .00 | .00 |
| 22 | .1163 | 1.5000 | 10.00 | .00 | .00 |
| 23 | .3649 | 1.5000 | 15.00 | .00 | .00 |
| 24 | .6642 | 1.5000 | 20.00 | .00 | .00 |
| 25 | .7942 | 1.5000 | 25.00 | .00 | .00 |
| 26 | .7405 | 1.5000 | 30.00 | .00 | .00 |
| 27 | .4946 | 1.5000 | 35.00 | .00 | .00 |
| 28 | .1951 | 1.5000 | 40.00 | .00 | .00 |
| 29 | .0556 | 1.5000 | 45.00 | .00 | .00 |
| 30 | .0308 | 1.5000 | 50.00 | .00 | .00 |
| 31 | .0336 | 2.0000 | 5.00 | .00 | .00 |
| 32 | .0921 | 2.0000 | 10.00 | .00 | .00 |
| 33 | .2546 | 2.0000 | 15.00 | .00 | .00 |
| 34 | .5023 | 2.0000 | 20.00 | .00 | .00 |
| 35 | .6798 | 2.0000 | 25.00 | .00 | .00 |
| 36 | .6966 | 2.0000 | 30.00 | .00 | .00 |
| 37 | .5484 | 2.0000 | 35.00 | .00 | .00 |
| 38 | .3017 | 2.0000 | 40.00 | .00 | .00 |
| 39 | .1170 | 2.0000 | 45.00 | .00 | .00 |
| 40 | .0508 | 2.0000 | 50.00 | .00 | .00 |
| 41 | .6269 | 2.0000 | 30.00 | .00 | .00 |
| 42 | .7154 | 2.0000 | 30.00 | 2.00 | .00 |
| 43 | .4751 | 2.0000 | 30.00 | 4.00 | .00 |
| 44 | .4078 | 2.0000 | 30.00 | 6.00 | .00 |
| 45 | .2044 | 2.0000 | 30.00 | 8.00 | .00 |
| 46 | .1392 | 2.0000 | 30.00 | 10.00 | .00 |
| 47 | .0647 | 2.0000 | 30.00 | 12.00 | .00 |
| 48 | .0535 | 2.0000 | 30.00 | 14.00 | .00 |
| 49 | .0368 | 2.0000 | 30.00 | 16.00 | .00 |
| 50 | .0428 | 2.0000 | 30.00 | 18.00 | .00 |
| 51 | .0347 | 2.0000 | 30.00 | 20.00 | .00 |
| 52 | .7663 | 2.0000 | 30.00 | .00 | .00 |
| 53 | .6259 | 2.0000 | 30.00 | .00 | 2.00 |
| 54 | .7543 | 2.0000 | 30.00 | .00 | 4.00 |
| 55 | .5806 | 2.0000 | 30.00 | .00 | 6.00 |
| 56 | .5929 | 2.0000 | 30.00 | .00 | 8.00 |
| 57 | .3309 | 2.0000 | 30.00 | .00 | 10.00 |
| 58 | .2159 | 2.0000 | 30.00 | .00 | 12.00 |
| 59 | .0812 | 2.0000 | 30.00 | .00 | 14.00 |
| 60 | .0546 | 2.0000 | 30.00 | .00 | 16.00 |
| 61 | .0396 | 2.0000 | 30.00 | .00 | 18.00 |
| 62 | .0425 | 2.0000 | 30.00 | .00 | 20.00 |

RESULTS FOR EACH ITERATION STEP

| STEP | SSQ | R | MU | LAM | Dx | Dy | Dz |
|---|---|---|---|---|---|---|---|
| 0 | 3.40837 | 1.000 | .010 | .010 | 50.000 | 5.000 | 2.500 |
| 1 | 1.18791 | 2.078 | .124 | .035 | 66.485 | 9.622 | 2.111 |
| 2 | .44395 | 2.691 | .245 | .073 | 2.081 | 10.382 | 3.921 |
| 3 | .15055 | 2.568 | .429 | .114 | 6.229 | 7.595 | 3.754 |
| 4 | .05225 | 2.520 | .249 | .076 | 13.741 | 9.048 | 4.517 |
| 5 | .03761 | 2.501 | .125 | .054 | 18.994 | 9.807 | 4.852 |
| 6 | .03733 | 2.500 | .104 | .051 | 19.921 | 9.965 | 4.934 |
| 7 | .03733 | 2.500 | .102 | .051 | 19.957 | 9.977 | 4.949 |
| 8 | .03733 | 2.500 | .102 | .051 | 19.960 | 9.978 | 4.951 |
| 9 | .03733 | 2.500 | .102 | .051 | 19.961 | 9.979 | 4.952 |

CORRELATION MATRIX

| | R | MU | LAM | Dx | Dy | Dz |
|---|---|---|---|---|---|---|
| R | 1.0000 | | | | | |
| MU | .0128 | 1.0000 | | | | |
| LAM | .1296 | .7416 | 1.0000 | | | |
| Dx | .2004 | -.5500 | -.4640 | 1.0000 | | |
| Dy | .2004 | -.8408 | -.4095 | .2597 | 1.0000 | |
| Dz | -.0621 | .2403 | .2881 | -.1271 | -.0953 | 1.0000 |

r^2 FOR REGRESSION OF OBSERVED VS. PREDICTED VALUES = .993742

MEAN SQUARE FOR ERROR (MSE) = .000667

BIAS (%) = .00 VARIANCE (%) = 100.00

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

| VAR | NAME | VALUE | S.E.COEFF. | T-VALUE | 95% CONFIDENCE LIMITS LOWER | UPPER |
|---|---|---|---|---|---|---|
| 1 | R | 2.50022 | .0495 | 50.46 | 2.401 | 2.599 |
| 2 | MU | .10222 | .0548 | 1.87 | -.008 | .212 |
| 3 | LAM | .05055 | .0103 | 4.89 | .030 | .071 |
| 4 | Dx | 19.96057 | 1.5951 | 12.51 | 16.765 | 23.156 |
| 5 | Dy | 9.97853 | 1.1162 | 8.94 | 7.742 | 12.215 |
| 6 | Dz | 4.95181 | .0007 | 7023.24 | 4.950 | 4.953 |

| ----ORDERED BY COMPUTER INPUT----- | | | | --------ORDERED BY RESIDUALS------ | | | |
|---|---|---|---|---|---|---|---|
| | CONCENTRATION | | RESI- | | CONCENTRATION | | RESI- |
| NO | OBS | FITTED | DUAL | NO | OBS | FITTED | DUAL |
| 1 | .016 | .016 | .000 | 52 | .766 | .697 | .070 |
| 2 | .242 | .242 | .000 | 54 | .754 | .686 | .068 |
| 3 | .838 | .838 | .000 | 42 | .715 | .650 | .065 |
| 4 | .976 | .975 | .000 | 56 | .593 | .540 | .053 |
| 5 | .972 | .971 | .000 | 44 | .408 | .371 | .037 |
| 6 | .746 | .746 | .000 | 58 | .216 | .196 | .020 |
| 7 | .150 | .150 | .000 | 46 | .139 | .127 | .013 |
| 8 | .012 | .012 | .000 | 60 | .055 | .050 | .005 |
| 9 | .010 | .010 | .000 | 48 | .054 | .049 | .005 |
| 10 | .010 | .010 | .000 | 62 | .043 | .039 | .004 |
| 11 | .028 | .028 | .000 | 50 | .043 | .039 | .003 |
| 12 | .160 | .160 | .000 | 4 | .976 | .975 | .000 |
| 13 | .551 | .551 | .000 | 5 | .972 | .971 | .000 |
| 14 | .847 | .847 | .000 | 7 | .150 | .150 | .000 |
| 15 | .893 | .893 | .000 | 2 | .242 | .242 | .000 |
| 16 | .766 | .766 | .000 | 25 | .794 | .794 | .000 |
| 17 | .375 | .375 | .000 | 15 | .893 | .893 | .000 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 18 | .079 | .079 | .000 | 26 | .741 | .740 | .000 |
| 19 | .022 | .022 | .000 | 35 | .680 | .680 | .000 |
| 20 | .020 | .020 | .000 | 36 | .697 | .697 | .000 |
| 21 | .032 | .032 | .000 | 14 | .847 | .847 | .000 |
| 22 | .116 | .116 | .000 | 17 | .375 | .375 | .000 |
| 23 | .365 | .365 | .000 | 12 | .160 | .160 | .000 |
| 24 | .664 | .664 | .000 | 37 | .548 | .548 | .000 |
| 25 | .794 | .794 | .000 | 28 | .195 | .195 | .000 |
| 26 | .741 | .740 | .000 | 24 | .664 | .664 | .000 |
| 27 | .495 | .495 | .000 | 27 | .495 | .495 | .000 |
| 28 | .195 | .195 | .000 | 34 | .502 | .502 | .000 |
| 29 | .056 | .056 | .000 | 38 | .302 | .302 | .000 |
| 30 | .031 | .031 | .000 | 16 | .766 | .766 | .000 |
| 31 | .034 | .034 | .000 | 13 | .551 | .551 | .000 |
| 32 | .092 | .092 | .000 | 18 | .079 | .079 | .000 |
| 33 | .255 | .255 | .000 | 23 | .365 | .365 | .000 |
| 34 | .502 | .502 | .000 | 8 | .012 | .012 | .000 |
| 35 | .680 | .680 | .000 | 1 | .016 | .016 | .000 |
| 36 | .697 | .697 | .000 | 33 | .255 | .255 | .000 |
| 37 | .548 | .548 | .000 | 22 | .116 | .116 | .000 |
| 38 | .302 | .302 | .000 | 11 | .028 | .028 | .000 |
| 39 | .117 | .117 | .000 | 6 | .746 | .746 | .000 |
| 40 | .051 | .051 | .000 | 3 | .838 | .838 | .000 |
| 41 | .627 | .697 | -.070 | 10 | .010 | .010 | .000 |
| 42 | .715 | .650 | .065 | 9 | .010 | .010 | .000 |
| 43 | .475 | .528 | -.053 | 39 | .117 | .117 | .000 |
| 44 | .408 | .371 | .037 | 32 | .092 | .092 | .000 |
| 45 | .204 | .227 | -.023 | 21 | .032 | .032 | .000 |
| 46 | .139 | .127 | .013 | 29 | .056 | .056 | .000 |
| 47 | .065 | .072 | -.007 | 31 | .034 | .034 | .000 |
| 48 | .054 | .049 | .005 | 19 | .022 | .022 | .000 |
| 49 | .037 | .041 | -.004 | 20 | .020 | .020 | .000 |
| 50 | .043 | .039 | .003 | 40 | .051 | .051 | .000 |
| 51 | .035 | .039 | -.004 | 30 | .031 | .031 | .000 |
| 52 | .766 | .697 | .070 | 61 | .040 | .040 | -.001 |
| 53 | .626 | .695 | -.069 | 51 | .035 | .039 | -.004 |
| 54 | .754 | .686 | .068 | 49 | .037 | .041 | -.004 |
| 55 | .581 | .646 | -.065 | 47 | .065 | .072 | -.007 |
| 56 | .593 | .540 | .053 | 59 | .081 | .090 | -.009 |
| 57 | .331 | .368 | -.037 | 45 | .204 | .227 | -.023 |
| 58 | .216 | .196 | .020 | 57 | .331 | .368 | -.037 |
| 59 | .081 | .090 | -.009 | 43 | .475 | .528 | -.053 |
| 60 | .055 | .050 | .005 | 55 | .581 | .646 | -.065 |
| 61 | .040 | .040 | -.001 | 53 | .626 | .695 | -.069 |
| 62 | .043 | .039 | .004 | 41 | .627 | .697 | -.070 |

END OF PROBLEM

```
*******************************************************************
*                                                                 *
*                            3DADE                                *
*                                                                 *
*      ANALYTICAL SOLUTIONS FOR SOLUTE TRANSPORT IN 3-D SEMI-     *
*        INFINITE POROUS MEDIA (WRR 27(10):2719-2733, 1991)       *
*         WITH FITTING BY NONLINEAR LEAST SQUARES ANALYSIS        *
*                                                                 *
*                                                                 *
*     4: LONGITUDINAL AND TRANSVERSE PROFILE                      *
*                                                                 *
*     MODEL 7                      FIRST-TYPE INLET CONDITION     *
*     SCENARIO 4: SOLUTE APPLICATION FROM A CIRCULAR              *
*                 SOURCE AT THE SOIL SURFACE                      *
*                                                                 *
*******************************************************************
```

INITIAL ESTIMATES OF MODEL PARAMETERS

| NAME | VALUE | FITTING |
|---|---|---|
| V | 20.00 | - |
| R | 1.00 | - |
| To | .10 | + |
| MU | .00 | - |
| LAM | .00 | - |
| Dx | 20.00 | + |
| Dr | 20.00 | + |

CONSTANTS

| NAME | VALUE |
|---|---|
| Co | 1.00 |
| a | 5.00 |

OBSERVED CONCENTRATIONS

| NO | C | t | x | r |
|---|---|---|---|---|
| 1 | .0563 | .5000 | 2.00 | .00 |
| 2 | .1476 | .5000 | 4.00 | .00 |
| 3 | .2499 | .5000 | 6.00 | .00 |
| 4 | .3262 | .5000 | 8.00 | .00 |
| 5 | .3489 | .5000 | 10.00 | .00 |
| 6 | .3164 | .5000 | 12.00 | .00 |
| 7 | .2492 | .5000 | 14.00 | .00 |
| 8 | .1736 | .5000 | 16.00 | .00 |
| 9 | .1085 | .5000 | 18.00 | .00 |
| 10 | .0614 | .5000 | 20.00 | .00 |
| 11 | .3402 | .5000 | 10.00 | 1.00 |
| 12 | .3144 | .5000 | 10.00 | 2.00 |
| 13 | .2733 | .5000 | 10.00 | 3.00 |
| 14 | .2212 | .5000 | 10.00 | 4.00 |
| 15 | .1648 | .5000 | 10.00 | 5.00 |
| 16 | .1120 | .5000 | 10.00 | 6.00 |
| 17 | .0690 | .5000 | 10.00 | 7.00 |
| 18 | .0384 | .5000 | 10.00 | 8.00 |
| 19 | .0193 | .5000 | 10.00 | 9.00 |
| 20 | .0088 | .5000 | 10.00 | 10.00 |

RESULTS FOR EACH ITERATION STEP

| STEP | SSQ | To | Dx | Dr |
|---|---|---|---|---|
| 0 | .46553 | .100 | 20.000 | 20.000 |
| 1 | .05175 | .146 | 21.778 | .997 |
| 2 | .00836 | .194 | 31.486 | 3.175 |
| 3 | .00234 | .213 | 33.662 | 6.352 |
| 4 | .00006 | .244 | 38.466 | 9.553 |
| 5 | .00000 | .250 | 39.956 | 9.983 |
| 6 | .00000 | .250 | 40.007 | 9.999 |
| 7 | .00000 | .250 | 40.007 | 9.999 |

CORRELATION MATRIX

| | To | Dx | Dr |
|---|---|---|---|
| To | 1.0000 | | |
| Dx | .8246 | 1.0000 | |
| Dr | .9360 | .6764 | 1.0000 |

r^2 FOR REGRESSION OF OBSERVED VS. PREDICTED VALUES = 1.000000

MEAN SQUARE FOR ERROR (MSE) = .000000

BIAS (%) = .01 VARIANCE (%) = 99.99

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

| VAR | NAME | VALUE | S.E.COEFF. | T-VALUE | 95% CONFIDENCE LIMITS LOWER | UPPER |
|---|---|---|---|---|---|---|
| 1 | To | .25001 | .0000 | 12366.59 | .250 | .250 |
| 2 | Dx | 40.00717 | .0054 | 7360.86 | 39.996 | 40.019 |
| 3 | Dr | 9.99935 | .0022 | 4446.62 | 9.995 | 10.004 |

| ----ORDERED BY COMPUTER INPUT----- | | | | --------ORDERED BY RESIDUALS------ | | | |
|---|---|---|---|---|---|---|---|
| NO | CONCENTRATION OBS | FITTED | RESI-DUAL | NO | CONCENTRATION OBS | FITTED | RESI-DUAL |
| 1 | .056 | .056 | .000 | 14 | .221 | .221 | .000 |
| 2 | .148 | .148 | .000 | 2 | .148 | .148 | .000 |
| 3 | .250 | .250 | .000 | 15 | .165 | .165 | .000 |
| 4 | .326 | .326 | .000 | 20 | .009 | .009 | .000 |
| 5 | .349 | .349 | .000 | 11 | .340 | .340 | .000 |
| 6 | .316 | .316 | .000 | 12 | .314 | .314 | .000 |
| 7 | .249 | .249 | .000 | 1 | .056 | .056 | .000 |
| 8 | .174 | .174 | .000 | 9 | .109 | .108 | .000 |
| 9 | .109 | .108 | .000 | 13 | .273 | .273 | .000 |
| 10 | .061 | .061 | .000 | 10 | .061 | .061 | .000 |
| 11 | .340 | .340 | .000 | 7 | .249 | .249 | .000 |
| 12 | .314 | .314 | .000 | 19 | .019 | .019 | .000 |
| 13 | .273 | .273 | .000 | 8 | .174 | .174 | .000 |
| 14 | .221 | .221 | .000 | 4 | .326 | .326 | .000 |
| 15 | .165 | .165 | .000 | 18 | .038 | .038 | .000 |
| 16 | .112 | .112 | .000 | 5 | .349 | .349 | .000 |
| 17 | .069 | .069 | .000 | 16 | .112 | .112 | .000 |
| 18 | .038 | .038 | .000 | 17 | .069 | .069 | .000 |
| 19 | .019 | .019 | .000 | 6 | .316 | .316 | .000 |
| 20 | .009 | .009 | .000 | 3 | .250 | .250 | .000 |

END OF PROBLEM

# APPENDIX G: LISTING OF 3DADE.FOR

```
C     ****************************************************************
C     *                                                              *
C     *                          3DADE                               *
C     *                                                              *
C     *     ANALYTICAL SOLUTIONS FOR SOLUTE TRANSPORT IN 3-D SEMI-   *
C     *      INFINITE POROUS MEDIA (WRR 27(10):2719-2733, 1991)      *
C     *       WITH FITTING BY NONLINEAR LEAST SQUARES ANALYSIS       *
C     *                                                              *
C     *             FEIKE J. LEIJ AND SCOTT BRADFORD                 *
C     *                                                              *
C     *                 U.S. SALINITY LABORATORY                     *
C     *                   4500 GLENWOOD DRIVE                        *
C     *                   RIVERSIDE, CA 92501                        *
C     *                                                              *

C     *                   PHONE (714) 369-4846                       *
C     *                   FAX   (714) 369-4818                       *
C     *                                                              *
C     *                      VERSION  12/93                          *
C     ****************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      LOGICAL PROD
      PARAMETER (NCON=250,ZIP=1.0D-08)
      COMMON NPAR,C,MODEL,NIV,INDEX
      DIMENSION Y(NCON),X(4,NCON),F(NCON),R(NCON),DELZ(NCON,8),B(16),
     $TH(16),P(8),PHI(8),Q(8),LSORT(NCON),TB(16),A(8,8),D(8,8),INDEX(8),
     $DX(4),XLOW(4),XUP(4),NXST(4),C(5),E(8),DEV(NCON)
      CHARACTER TITLE*60,BI(8)*10,TBI(8)*10,CN(5)*5,VN(4)*5,FILENAME*15,
     $JUNK*60
      DATA TBI/'V','R','To','MU','LAM','Dx',' ','Dz'/,
     $STOPCR/0.001/,MAXTRY/50/
      DATA VN/'t','x',' ','z'/,CN/'Co','a','b','x1','x2'/
C
C     --- OPEN I/O FILES ---
      WRITE(*, 150)
      READ(*, 160) FILENAME
      IF (FILENAME.EQ.'  ') FILENAME='3DADE.IN'
      OPEN(5, FILE=FILENAME, STATUS='OLD')
C
      WRITE(*, 170)
      READ(*,160) FILENAME
      IF (FILENAME.EQ.'  ') FILENAME='3DADE.OUT'
      OPEN(7, FILE=FILENAME, STATUS='UNKNOWN')
C
C     --- READ MODEL ---
      READ(5,201) JUNK
      READ(5,203) MODEL,MIT,IND,NGC
C
C     --- INITIALIZATIONS ---
      DO 2 I=1,8
    2  BI(I)=TBI(I)
      DO 3 I=1,4,3
       DX(I)=0.0
       XLOW(I)=0.0
       XUP(I)=1.0
    3  NXST(I)=1.0
      IF ((MODEL.GE.1.AND.MODEL.LE.6).OR.MODEL.EQ.11.OR.MODEL.EQ.12)THEN
       NIV=4
       NPAR=16
       BI(7)='Dy'
       VN(3)='y'
      ELSE IF ((MODEL.GE.7.AND.MODEL.LE.10).OR.MODEL.EQ.13) THEN
       NIV=3
```

```
        NPAR=15
        BI(7)='Dr'
        VN(3)='r'
       ENDIF
       PROD=.TRUE.
C
C      --- READ INPUT FILE ---
       READ(5,201) TITLE
       READ(5,201) JUNK
       READ(5,202) (B(I),I=9,13)
       READ(5,203) (INDEX(I),I=1,5)
       READ(5,201) JUNK
       READ(5,202) (B(I),I=14,NPAR)
       READ(5,203) (INDEX(I),I=6,NPAR-8)
       READ(5,201) JUNK
       READ(5,202) (C(I),I=1,5)
C
C      --- DIRECT PROBLEM ---
       IF (IND.EQ.0) THEN
        NOB=1
        DO 4 I=1,NPAR-8
   4     INDEX(I)=0
C
        DO 5 I=1,4
         IF ((MODEL.GT.10.AND.I.EQ.1).OR.
     $   (((MODEL.GE.7.AND.MODEL.LE.10).OR.MODEL.EQ.13).AND.I.EQ.4)) THEN
          READ(5,201) JUNK
          READ(5,205)
          GOTO 5
         ENDIF
         READ(5,201) JUNK
         READ(5,202) DX(I),XLOW(I),XUP(I)
    5   CONTINUE
        GOTO 8
       ENDIF
C
C      --- INDIRECT PROBLEM ---
       IF (MODEL.GT.10) INDEX(2)=0
       IF (MODEL.EQ.5 .OR. MODEL.EQ.6 .OR. MODEL.GT.8) INDEX(3)=0
       IF (MODEL.GT.10) INDEX(4)=0
       IF (MODEL.GT.10) INDEX(5)=0
       IF (MODEL.GT.10) INDEX(6)=0
C
       NOB=0
       DO 6 I=1,NCON
        IF(MODEL.GE.11) THEN
         READ(5,*,END=8) Y(I),(X(J,I),J=2,NIV)
        ELSE
         READ(5,*,END=8) Y(I),(X(J,I),J=1,NIV)
        ENDIF
    6  NOB=NOB+1
C
C      --- ERROR MESSAGES ---
    8  IF (MODEL.GT.13.OR.MODEL.LT.1)
     $  STOP 'LINE 2 INPUT FILE : MODEL NUMBER 1-13'
       IF (MIT.LT.0)
     $  STOP 'LINE 2 INPUT FILE : MIT >= 0'
       IF (MODEL.LE.10.AND.B(10).LE.0.0) STOP 'LINE 4 INPUT FILE : R > 0'
       IF (B(9).LT.0.0) STOP 'LINE 4 INPUT FILE : V >=0'
       IF (MODEL.LE.4 .OR. MODEL.EQ.7 .OR. MODEL.EQ.8) THEN
        IF (B(11).LT.0.0) STOP 'LINE 4 INPUT FILE : To >= 0'
       ENDIF
       IF ((MODEL.GE.1.AND.MODEL.LE.6).AND.
     $ (B(14).LE.0.0.OR.B(15).LE.0.0.OR.B(16).LE.0.0))
     $  STOP 'LINE 6 INPUT FILE : Dx, Dy, Dz > 0'
```

```
      IF ((MODEL.GE.7.AND.MODEL.LE.10).AND.
     $ (B(14).LE.0.0.OR.B(15).LE.0.0))
     $  STOP 'LINE 6 INPUT FILE : Dx, Dr > 0'
      IF ((MODEL.EQ.11.OR.MODEL.EQ.12).AND.
     $ (B(15).LE.0.0.OR.B(16).LE.0.0))
     $  STOP 'LINE 6 INPUT FILE : Dy, Dz > 0'
      IF (MODEL.EQ.13.AND.B(15).LE.0.0)
     $  STOP 'LINE 6 INPUT FILE : Dr > 0'
      IF (C(1).LT.0.0)
     $  STOP 'LINE 8 INPUT FILE : Co >=0'
      IF ((MODEL.EQ.3.OR.MODEL.EQ.4.OR.MODEL.EQ.12) .AND.
     $  (C(2).LT.0.0 .OR. C(3).LT.0.0))
     $  STOP 'LINE 8 INPUT FILE : a,b >= 0'
      IF ((MODEL.EQ.5.OR.MODEL.EQ.6) .AND.
     $  (C(2).LT.0.0.OR.C(3).LT.0.0.OR.C(4).LT.0.0.OR.C(5).LT.0.0))
     $  STOP 'LINE 8 INPUT FILE : a,b,x1,x2 >= 0'
      IF ((MODEL.EQ.7.OR.MODEL.EQ.8.OR.MODEL.EQ.13) .AND. C(2).LT.0.0)
     $  STOP 'LINE 8 INPUT FILE : a >= 0'
      IF ((MODEL.EQ.9.OR.MODEL.EQ.10) .AND.
     $  (C(2).LT.0.0.OR.C(4).LT.0.0.OR.C(5).LT.0.0))
     $  STOP 'LINE 8 INPUT FILE : a,x1,x2 >= 0'
      IF ((MODEL.EQ.5.OR.MODEL.EQ.6.OR.MODEL.EQ.9.OR.MODEL.EQ.10)
     $  .AND. C(4).GT.C(5))
     $  STOP 'LINE 8 INPUT FILE : x1 <= x2'
      IF(IND.EQ.1) GOTO 11
      DO 9 I=1,2
    9 IF (XLOW(I).LT.0.0.OR.XUP(I).LT.0.0)
     $  STOP 'INPUT ERROR GRID SYSTEM : x,t >= 0'
      DO 10 I=1,4
      IF (DX(I).LT.0.0)
     $  STOP 'INPUT ERROR GRID SYSTEM : INCREMENTS MUST BE POSITIVE'
   10 IF (XLOW(I).GT.XUP(I))
     $  STOP 'INPUT ERROR GRID SYSTEM : UPPER AND LOWER LIMITS'
      IF (((MODEL.GE.7.AND.MODEL.LE.10).OR.MODEL.EQ.13).AND.
     $XLOW(3).LT.0.0)
     $  STOP 'INPUT ERROR GRID SYSTEM : r >= 0'
      IF(IND.EQ.0) GOTO 14
   11 IF (INDEX(1).EQ.1.AND.INDEX(2).EQ.1.AND.INDEX(6).EQ.1)
     $  STOP 'EITHER v, R, OR Dx SHOULD BE FIXED'
      NINDEX = 0
      DO 12 I=1,8
      IF (INDEX(I).EQ.1.AND.ABS(B(I+8)).LE.ZIP)
     $  STOP 'INITIAL ESTIMATE OF FITTED VARIABLE CANNOT BE ZERO'
      IF (INDEX(I).EQ.1) NINDEX=NINDEX+1
   12 CONTINUE
      IF (NINDEX.EQ.1) STOP 'AT LEAST TWO VARIABLES MUST BE FITTED'
       DO 13 I=1,NOB
   13   IF (Y(I).LT.0.0.OR.X(1,I).LT.0.0.OR.X(2,I).LT.0.0)
     $   STOP 'INPUT ERROR OBSERVATIONS - C/Co, t, AND x >= 0.0'
C
C     --- CLEAR SCREEN AND WRITE TITLE ---
   14 WRITE(*,180)
      IF (IND.EQ.0) WRITE(*,190) FILENAME
      IF (IND.EQ.1) WRITE(*,191) FILENAME
      WRITE(*,195)
C
C     --- START MAIN PROGRAM ---
      WRITE(7,300)
      WRITE(7,302) TITLE
C
C     --- WRITE MODEL TYPE ---
      IF (MODEL.EQ.1)  WRITE(7,304)
      IF (MODEL.EQ.2)  WRITE(7,306)
      IF (MODEL.EQ.3)  WRITE(7,308)
      IF (MODEL.EQ.4)  WRITE(7,310)
```

```
      IF (MODEL.EQ.5)  WRITE(7,312)
      IF (MODEL.EQ.6)  WRITE(7,314)
      IF (MODEL.EQ.7)  WRITE(7,316)
      IF (MODEL.EQ.8)  WRITE(7,318)
      IF (MODEL.EQ.9)  WRITE(7,320)
      IF (MODEL.EQ.10) WRITE(7,322)
      IF (MODEL.EQ.11) WRITE(7,324)
      IF (MODEL.EQ.12) WRITE(7,326)
      IF (MODEL.EQ.13) WRITE(7,328)
C
C     --- WRITE PARAMETER VALUES AND MODEL CONSTANTS ---
      IF (IND.EQ.0) WRITE(7,330)
      IF (IND.EQ.1) WRITE(7,331)
      DO 15 I=9,NPAR
       IF ((MODEL.EQ.5.OR.MODEL.EQ.6) .AND. I.EQ.11) GOTO 15
       IF ((MODEL.EQ.9.OR.MODEL.EQ.10) .AND. I.EQ.11) GOTO 15
       IF ((MODEL.EQ.11.OR.MODEL.EQ.12).AND.(I.GT.9.AND.I.LT.15))GOTO 15
       IF (MODEL.EQ.13 .AND. (I.GT.9.AND.I.LT.15)) GOTO 15
       IF (IND.EQ.0) WRITE(7,336) BI(I-8),B(I)
       IF (IND.EQ.1) THEN
  IF(INDEX(I-8).EQ.0) THEN
          WRITE(7,332) BI(I-8),B(I),'-'
  ELSE
          WRITE(7,332) BI(I-8),B(I),'+'
         ENDIF
       ENDIF
   15 CONTINUE
C
      WRITE(7,334)
      DO 16 I=1,5
       IF ((MODEL.LE.2.OR.MODEL.EQ.11).AND.I.GT.1) GOTO 16
       IF ((MODEL.EQ.3.OR.MODEL.EQ.4.OR.MODEL.EQ.12).AND.I.GT.3) GOTO 16
       IF ((MODEL.EQ.7.OR.MODEL.EQ.8.OR.MODEL.GE.13).AND.I.GT.2) GOTO 16
       IF ((MODEL.EQ.9.OR.MODEL.EQ.10).AND.I.EQ.3) GOTO 16
       WRITE(7,336) CN(I),C(I)
   16 CONTINUE
C
C     --- CALCULATE NODE SPACING ---
      IF (IND.EQ.0) THEN
      WRITE(7,338)
      DO 17 J=1,NIV
       I=J
       IF (MODEL.GT.10) I=J+1
       IF (ABS(DX(I)).LE.ZIP) THEN
        NXST(I)=1
       ELSE
        NXST(I)=ZIP+(XUP(I)+DX(I)-XLOW(I))/DX(I)
       ENDIF
       WRITE(7,340) VN(I),DX(I),XLOW(I),XUP(I)
       IF (MODEL.GT.10.AND.I.EQ.NIV) GOTO 18
   17 CONTINUE
C
   18 IF (MODEL.LE.6.) THEN
       WRITE(7,342) CHAR(12)
      ELSE IF (MODEL.GE.7 .AND. MODEL.LE.10) THEN
       WRITE(7,343) CHAR(12)
      ELSE IF (MODEL.EQ.11 .OR. MODEL.EQ.12) THEN
       WRITE(7,344) CHAR(12)
      ELSE
       WRITE(7,345) CHAR(12)
      ENDIF
C
      NUM=0
      DO 19 I=1,NXST(1)
       X(1,1)=XLOW(1)+(I-1)*DX(1)
```

```
      DO 19 J=1,NXST(2)
       X(2,1)=XLOW(2)+(J-1)*DX(2)
       PROD=.TRUE.
       DO 19 K=1,NXST(3)
        X(3,1)=XLOW(3)+(K-1)*DX(3)
        DO 19 L=1,NXST(4)
         X(4,1)=XLOW(4)+(L-1)*DX(4)
         NUM=NUM+1
         CALL MODELS(B,Y,NOB,NCON,X,NGC,PROD)
         PROD=.FALSE.
         IF (C(1).GT.0.0) YY=Y(1)/C(1)
      IF (MODEL.LE.10) WRITE(7,346) NUM,Y(1),YY,(X(JJ,1), JJ=1,NIV)
19    IF (MODEL.GT.10) WRITE(7,346) NUM,Y(1),YY,(X(JJ,1), JJ=2,NIV)
      GO TO 119
     ENDIF
C
C    --- ELSE WRITE EXPERIMENTAL DATA ---
     II=1
     IF (MODEL.LE.6.) THEN
      WRITE(7,347) CHAR(12)
     ELSE IF (MODEL.GE.7 .AND. MODEL.LE.10) THEN
      WRITE(7,348) CHAR(12)
     ELSE IF (MODEL.EQ.11 .OR. MODEL.EQ.12) THEN
      WRITE(7,349) CHAR(12)
     ELSE
      WRITE(7,350) CHAR(12)
     ENDIF
     DO 24 I=1,NOB
      IF (MODEL.LE.10) WRITE(7,346) I,Y(I),(X(J,I), J=1,NIV)
24    IF (MODEL.GT.10) WRITE(7,346) I,Y(I),(X(J,I), J=2,NIV)
C
C    --- BEGIN FITTING ---
     NP=0
     DO 26 I=9,NPAR
      TB(I)=B(I)
      IF (INDEX(I-8).EQ.0) GO TO 26
      NP=NP+1
      BI(NP)=BI(I-8)
      B(NP)=B(I)
      TB(NP)=B(I)
      TH(NP)=B(NP)
26   TH(I)=B(I)
C
C    ------
     GA=0.02
     NIT=0
     CALL MODELS(TH,F,NOB,NCON,X,NGC,PROD)
     SSQ=0.
     DO 32 I=1,NOB
      R(I)=Y(I)-F(I)
32    SSQ=SSQ+R(I)*R(I)
     WRITE(7,357) (BI(J),J=1,NP)
     WRITE(7,358) NIT,SSQ,(B(I),I=1,NP)
C
C    --- BEGIN OF ITERATION ---
34   NIT=NIT+1
     NTRIAL=0
     GA=0.1*GA
     DO 38 J=1,NP
     TEMP=TH(J)
     TH(J)=1.01*TH(J)
     Q(J)=0
     CALL MODELS(TH,DELZ(1,J),NOB,NCON,X,NGC,PROD)
     DO 36 I=1,NOB
      DELZ(I,J)=DELZ(I,J)-F(I)
```

```
   36  Q(J)=Q(J)+DELZ(I,J)*R(I)
      Q(J)=100.*Q(J)/TH(J)
C
C     --- Q=XT*R (STEEPEST DESCENT) ---
   38 TH(J)=TEMP
      DO 44 I=1,NP
      DO 42 J=1,I
      SUM=0
      DO 40 K=1,NOB
   40  SUM=SUM+DELZ(K,I)*DELZ(K,J)
      D(I,J)=10000.*SUM/(TH(I)*TH(J))
   42 D(J,I)=D(I,J)
   44 E(I)=DSQRT(D(I,I))
   50 DO 52 I=1,NP
       DO 52 J=1,NP
   52   A(I,J)=D(I,J)/(E(I) * E(J))
C
C     --- A IS THE SCALED MOMENT MATRIX ---
      DO 54 I=1,NP
       P(I)=Q(I)/E(I)
       PHI(I)=P(I)
   54  A(I,I)=A(I,I)+GA
      CALL MATINV(A,NP,P)
C
C     --- P/E IS THE CORRECTION VECTOR ---
      STEP=1.0
   56 DO 58 I=1,NP
   58  TB(I)=P(I)*STEP/E(I)+TH(I)
      DO 62 I=1,NP
       IF (TH(I)*TB(I)) 66,66,62
   62 CONTINUE
      SUMB=0
      CALL MODELS(TB,F,NOB,NCON,X,NGC,PROD)
      DO 64 I=1,NOB
       R(I)=Y(I)-F(I)
   64  SUMB=SUMB+R(I)*R(I)
   66 SUM1=0.0
      SUM2=0.0
      SUM3=0.0
      DO 68 I=1,NP
       SUM1=SUM1+P(I)*PHI(I)
       SUM2=SUM2+P(I)*P(I)
   68  SUM3=SUM3+PHI(I)*PHI(I)
      ARG=SUM1/DSQRT(SUM2*SUM3)
      ARG1=0.
      IF (NP.GT.1) ARG1=DSQRT(1.-ARG*ARG)
      ANGLE=57.29578*DATAN2(ARG1,ARG)
C
C     ------
      DO 72 I=1,NP
       IF (TH(I)*TB(I)) 74,74,72
   72 CONTINUE
      NTRIAL=NTRIAL+1
      IF(NTRIAL.GT.MAXTRY) GO TO 95
      IF (SUMB/SSQ-1.0) 80,80,74
   74 IF (ANGLE-30.0) 76,76,78
   76 STEP=0.5*STEP
      GOTO 56
   78 GA=10.*GA
      GOTO 50
C
C     --- PRINT COEFFICIENTS AFTER EACH ITERATION ---
   80 CONTINUE
      DO 82 I=1,NP
   82  TH(I)=TB(I)
```

```
      WRITE(7,358) NIT,SUMB,(TH(I),I=1,NP)
      DO 86 I=1,NP
       IF(DABS(P(I)*STEP/E(I))/(1.0D-20+DABS(TH(I)))-STOPCR) 86,86,94
   86 CONTINUE
      GOTO 96
   94 SSQ=SUMB
      IF (NIT.LT.MIT) GOTO 34
      IF (NIT.EQ.MIT) WRITE(7,353) NIT
      GOTO 96
   95 WRITE(7,354) MAXTRY
C
C     --- END OF ITERATION LOOP ---
   96 CONTINUE
      CALL MATINV(D,NP,P)
C
C     --- WRITE CORRELATION MATRIX ---
      DO 98 I=1,NP
   98  E(I)=DSQRT(DMAX1(D(I,I),1.D-20))
      WRITE(7,359) (BI(I),I=1,NP)
      DO 102 I=1,NP
       DO 100 J=1,I
  100   A(J,I)=D(J,I)/(E(I)*E(J))
  102  WRITE(7,360) BI(I),(A(J,I),J=1,I)
C
C     ----- CALCULATE r2 OF FITTED VS OBSERVED CONCENTRATION VALUES -----
      AVC=0.
      AVCDEV=0.
      IF(NOB.GT.0) THEN
       DO 103 I=1,NOB
        DEV(I)=Y(I)-F(I)
        AVC=AVC+Y(I)
  103   AVCDEV=AVCDEV+DEV(I)
       AVC=AVC/NOB
       AVCDEV=AVCDEV/NOB
C
       SUM1=0.
       SUM2=0.
       VARI=0.
       DO 104 I=1,NOB
        SUM1=SUM1+DEV(I)**2
        SUM2=SUM2+(Y(I)-AVC)**2
  104  VARI=VARI+(DEV(I)-AVCDEV)**2
       RSQ=1-SUM1/SUM2
       WRITE(7,355) RSQ
C
       IF(NOB.GT.NP) THEN
        UMSE=SUM1/(NOB-NP)
        WRITE(7,366) UMSE
       ENDIF
       IF(NOB.GT.0) THEN
        VARI=100*VARI/SUM1
        BIAS=100*NOB*AVCDEV**2/SUM1
        WRITE(7,367) BIAS,VARI
       ENDIF
      ENDIF
C
C     --- CALCULATE 95% CONFIDENCE INTERVAL ---
      Z=1./FLOAT(NOB-NP)
      SDEV=DSQRT(Z*SUMB)
      TVAR=1.96+Z*(2.3779+Z*(2.7135+Z*(3.187936+2.466666*Z**2)))
      WRITE(7,361)
      DO 108 I=1,NP
       SECOEF=E(I)*SDEV
       TVALUE=TH(I)/SECOEF
       TSEC=TVAR*SECOEF
```

```
       TMCOE=TH(I)-TSEC
       TPCOE=TH(I)+TSEC
  108  WRITE(7,362) I,BI(I),TH(I),SECOEF,TVALUE,TMCOE,TPCOE
C
C      --- PREPARE FINAL OUTPUT ---
      LSORT(1)=1
      DO 116 J=2,NOB
       TEMP=R(J)
       K=J-1
       DO 111 L=1,K
        LL=LSORT(L)
        IF(TEMP-R(LL)) 112,112,111
  111  CONTINUE
       LSORT(J)=J
       GO TO 116
  112  KK=J
  113  KK=KK-1
       LSORT(KK+1)=LSORT(KK)
       IF(KK-L) 115,115,113
  115  LSORT(L)=J
  116 CONTINUE
      WRITE(7,363)
      DO 118 I=1,NOB
      J=LSORT(NOB+1-I)
  118 WRITE(7,364) I,Y(I),F(I),R(I),J,Y(J),F(J),R(J)
  119 WRITE(7,365)
C
 C     --- END OF PROBLEM ---
  150 FORMAT(' Enter input file name (default = 3DADE.IN)')
  160 FORMAT(A15)
  170 FORMAT(' Enter output file name (default = 3DADE.OUT)')
  180 FORMAT(////////////////)
  190 FORMAT(//5X,67(1H*)/5X,1H*,65X,1H*/5X,1H*,30X,'3DADE',30X,1H*/5X,1
     $H*,65X,1H*/5X,1H*,4X,'PLEASE WAIT - The concentrations are being c
     $alculated and',4X,1H*/5x,1H*,18X,'written to ',A15,21X,1H*/,5X,1H*
     $,65X,1H*)
  191 FORMAT(//5X,67(1H*)/5X,1H*,65X,1H*/5X,1H*,30X,'3DADE',30X,1H*/5X,1
     $H*,65X,1H*/5X,1H*,2X,'PLEASE WAIT - The observed concentrations ar
     $e being fitted and',1X,1H*/5x,1H*,16X,'written to ',A15,23X,1H*/,5
     $X,1H*,65X,1H*)
  195 FORMAT(5X,67(1H*),///)
  200 FORMAT(5I5)
  201 FORMAT(A60)
  202 FORMAT(7F10.2)
  203 FORMAT(7I10)
  205 FORMAT()
  300 FORMAT(//5X,67(1H*)/5X,1H*,65X,1H*/5X,1H*,30X,'3DADE',30X,1H*/5X,
     $1H*,65X,1H*/5X,1H*,6X,'ANALYTICAL SOLUTIONS FOR SOLUTE TRANSPORT I
     $N 3-D SEMI-',5X,1H*/5X,1H*,8X,'INFINITE POROUS MEDIA (WRR 27(10):2
     $719-2733, 1991)',7X,1H*/5X,1H*,9X,'WITH FITTING BY NONLINEAR LEAST
     $ SQUARES ANALYSIS',8X,1H*/5X,1H*,65X,1H*/5X,1H*,65X,1H*)
  302 FORMAT(5X,1H*,5X,A60,1H*/5X,1H*,65X,1H*)
  304 FORMAT(5X,1H*,5X,'MODEL 1                      FIRST-TYPE INLET CO
     $NDITION',5X,1H*/5X,1H*,5X,'SCENARIO 1: SOLUTE APPLICATION FROM A S
     $EMI-INFINITE',9X,1H*/5X,1H*,17X,'QUADRANT OF AN INFINITE SOIL SURF
     $ACE',12X,1H*/5X,1H*,65X,1H*/5X,67(1H*))
  306 FORMAT(5X,1H*,5X,'MODEL 2                      THIRD-TYPE INLET CO
     $NDITION',5X,1H*/5X,1H*,5X,'SCENARIO 1: SOLUTE APPLICATION FROM A S
     $EMI-INFINITE',9X,1H*/5X,1H*,17X,'QUADRANT OF AN INFINITE SOIL SURF
     $ACE',12X,1H*/5X,1H*,65X,1H*/5X,67(1H*))
  308 FORMAT(5X,1H*,5X,'MODEL 3                      FIRST-TYPE INLET CO
     $NDITION',5X,1H*/5X,1H*,5X,'SCENARIO 2: SOLUTE APPLICATION FROM A R
     $ECTANGULAR',11X,1H*/5X,1H*,17X,'SOURCE AT THE SOIL SURFACE',22X,1H
     $*/5X,1H*,65X,1H*/5X,67(1H*))
  310 FORMAT(5X,1H*,5X,'MODEL 4                      THIRD-TYPE INLET CO
```

```
     $NDITION',5X,1H*/5X,1H*,5X,'SCENARIO 2: SOLUTE APPLICATION FROM A R
     $ECTANGULAR',11X,1H*/5X,1H*,17X,'SOURCE AT THE SOIL SURFACE',22X,1H
     $*/5X,1H*,65X,1H*/5X,67(1H*))
 312 FORMAT(5X,1H*,5X,'MODEL 5                             FIRST-TYPE INLET CO
     $NDITION',5X,1H*/5X,1H*,5X,'SCENARIO 3: SOLUTE INITIALLY UNIFORMLY
     $DISTRIBUTED IN A',5X,1H*/5X,1H*,17X,'PARALLELEPIPEDAL REGION OF TH
     $E SOIL',13X,1H*/5X,1H*,65X,1H*/5X,67(1H*))
 314 FORMAT(5X,1H*,5X,'MODEL 6                             THIRD-TYPE INLET CO
     $NDITION',5X,1H*/5X,1H*,5X,'SCENARIO 3: SOLUTE INITIALLY UNIFORMLY
     $DISTRIBUTED IN A',5X,1H*/5X,1H*,17X,'PARALLELEPIPEDAL REGION OF TH
     $E SOIL',13X,1H*/5X,1H*,65X,1H*/5X,67(1H*))
 316 FORMAT(5X,1H*,5X,'MODEL 7                             FIRST-TYPE INLET CO
     $NDITION',5X,1H*/5X,1H*,5X,'SCENARIO 4: SOLUTE APPLICATION FROM A C
     $IRCULAR',14X,1H*/5X,1H*,17X,'SOURCE AT THE SOIL SURFACE',22X,1H*/5
     $X,1H*,65X,1H*/5X,67(1H*))
 318 FORMAT(5X,1H*,5X,'MODEL 8                             THIRD-TYPE INLET CO
     $NDITION',5X,1H*/5X,1H*,5X,'SCENARIO 4: SOLUTE APPLICATION FROM A C
     $IRCULAR',14X,1H*/5X,1H*,17X,'SOURCE AT THE SOIL SURFACE',22X,1H*/5
     $X,1H*,65X,1H*/5X,67(1H*))
 320 FORMAT(5X,1H*,5X,'MODEL 9                             FIRST-TYPE INLET CO
     $NDITION',5X,1H*/5X,1H*,5X,'SCENARIO 5: SOLUTE INITIALLY UNIFORMLY
     $DISTRIBUTED IN A',5X,1H*/5X,1H*,17X,'CYLINDRICAL REGION OF THE SOI
     $L',18X,1H*/5X,1H*,65X,1H*/5X,67(1H*))
 322 FORMAT(5X,1H*,5X,'MODEL 10                            THIRD-TYPE INLET CO
     $NDITION',5X,1H*/5X,1H*,5X,'SCENARIO 5: SOLUTE INITIALLY UNIFORMLY
     $DISTRIBUTED IN A',5X,1H*/5X,1H*,17X,'CYLINDRICAL REGION OF THE SOI
     $L',18X,1H*/5X,1H*,65X,1H*/5X,67(1H*))
 324 FORMAT(5X,1H*,5X,'MODEL 11                                        STEAD
     $Y STATE',5X,1H*/5X,1H*,5X,'SCENARIO 1: SOLUTE APPLICATION FROM A S
     $EMI-INFINITE',9X,1H*/5X,1H*,17X,'QUADRANT OF AN INFINITE SOIL SURF
     $ACE',12X,1H*/5X,1H*,65X,1H*/5X,67(1H*))
 326 FORMAT(5X,1H*,5X,'MODEL 12                                        STEAD
     $Y STATE',5X,1H*/5X,1H*,5X,'SCENARIO 2: SOLUTE APPLICATION FROM A R
     $ECTANGULAR',11X,1H*/5X,1H*,17X,'SOURCE AT THE SOIL SURFACE',22X,1H
     $*/5X,1H*,65X,1H*/5X,67(1H*))
 328 FORMAT(5X,1H*,5X,'MODEL 13                                        STEAD
     $Y STATE',5X,1H*/5X,1H*,5X,'SCENARIO 4: SOLUTE APPLICATION FROM A C
     $IRCULAR',14X,1H*/5X,1H*,17X,'SOURCE AT THE SOIL SURFACE',22X,1H*/5
     $X,1H*,65X,1H*/5X,67(1H*))
 330 FORMAT(//5X,'MODEL PARAMETERS'/5X,16(1H=)/5X,'NAME',11X,'VALUE')
 331 FORMAT(//5X,'INITIAL ESTIMATES OF MODEL PARAMETERS'/5X,37(1H=)/5X,
     $'NAME',11X,'VALUE',7X,'FITTING')
 332 FORMAT(5X,A5,5X,F10.2,10X,A1)
 334 FORMAT(//5X,'CONSTANTS'/5X,9(1H=)/5X,'NAME',11X,'VALUE')
 336 FORMAT(5X,A5,5X,F10.2)
 338 FORMAT(//5X,'INDEPENDENT VARIABLES'/5X,21(1H=)/5X,'VARIABLE',3X,'I
     $NCREMENT',8X,'MINIMUM',8X,'MAXIMUM')
 340 FORMAT(5X,A5,5X,F10.3,5X,F10.3,5X,F10.3)
 342 FORMAT(/A1/5X,'PREDICTED CONCENTRATIONS'/5X,24(1H=)/8X,'NO',8X,'C'
     $,9X,'C/Co',8X,'t',9X,'x',9X,'y',9X,'z')
 343 FORMAT(/A1/5X,'PREDICTED CONCENTRATIONS'/5X,24(1H=)/8X,'NO',8X,'C'
     $,9X,'C/Co',8X,'t',9X,'x',9X,'r')
 344 FORMAT(/A1/5X,'PREDICTED CONCENTRATIONS'/5X,24(1H=)/8X,'NO',8X,'C'
     $,9X,'C/Co',8X,'x',9X,'y',9X,'z')
 345 FORMAT(/A1/5X,'PREDICTED CONCENTRATIONS'/5X,24(1H=)/8X,'NO',8X,'C'
     $,9X,'C/Co',8X,'x',9X,'r')
 346 FORMAT(5X,I5,3X,2F10.4,5F10.2)
 347 FORMAT(/A1/5X,'OBSERVED CONCENTRATIONS'/5X,23(1H=)/8X,'NO',8X,'C',
     $9X,'t',11X,'x',9X,'y',9X,'z',9X)
 348 FORMAT(/A1/5X,'OBSERVED CONCENTRATIONS'/5X,23(1H=)/8X,'NO',8X,'C',
     $9X,'t',11X,'x',9X,'r',9X)
 349 FORMAT(/A1/5X,'OBSERVED CONCENTRATIONS'/5X,23(1H=)/8X,'NO',8X,'C',
     $9X,'x',11X,'y',9X,'z',9X)
 350 FORMAT(/A1/5X,'OBSERVED CONCENTRATIONS'/5X,23(1H=)/8X,'NO',8X,'C',
     $9X,'x',11X,'r',9X)
```

```
  353 FORMAT(/5X,'CONVERGENCE CRITERION NOT MET IN ',I2,' ITERATIONS')
  354 FORMAT(/5X,'NO FURTHER DECREASE IN SSQ OBTAINED AFTER ',I2,' TRIAL
     $S')
  355 FORMAT(//5X,'r^2 FOR REGRESSION OF OBSERVED VS. PREDICTED VALUES =
     $',F9.6/5X,51(1H=))
  357 FORMAT(//5X,'RESULTS FOR EACH ITERATION STEP'/5X,31(1H=)/5X,'STEP'
     $,6X,'SSQ',5X,7(3X,A3,2X))
  358 FORMAT(5X,I3,3X,F10.5,2X,7(F7.3,1X))
  359 FORMAT(//5X,'CORRELATION MATRIX'/5X,18(1H=)/8X,10(2X,A3,6X))
  360 FORMAT(3X,A3,10(2X,F7.4,2X))
  361 FORMAT(///5X,'NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS'/5X
     $,48(1H=)//54X,'95% CONFIDENCE LIMITS'/5X,'VAR',5X,'NAME',3X,'VALUE
     $',6X,'S.E.COEFF.',3X,'T-VALUE',5X,'LOWER',8X,'UPPER')
  362 FORMAT(5X,I2,7X,A3,F10.5,1X,F11.4,1X,F11.2,1X,F10.3,1X,F12.3)
  363 FORMAT(//5X,4(1H-),'ORDERED BY COMPUTER INPUT',5(1H-), 3X,8(1H-),'
     $ORDERED BY RESIDUALS',6(1H-)/11X,3X,'CONCENTRATION',4X,'RESI-',8X,
     $8X,'CONCENTRATION',4X,'RESI-'/6X,'NO',2X,5X,'OBS ',2X,'FITTED',4X,
     $'DUAL',9X,'NO',1X,6X,'OBS ',2X,'FITTED',4X,'DUAL')
  364 FORMAT(5X,I3,3X,3F8.3,8X,I3,3X,3F8.3)
  365 FORMAT(///5X,'END OF PROBLEM'/5X,14(1H=))
  366 FORMAT(/5X,'MEAN SQUARE FOR ERROR (MSE) =',F11.6/5X,27(1H=))
  367 FORMAT(/5X,'BIAS (%)       =',F8.2,5X,'VARIANCE (%)      =',F8.2)
C
      CLOSE(5)
      CLOSE(7)
C
      STOP
      END
C
C     ------------
      SUBROUTINE MATINV(A,NP,B)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION A(8,8),B(16),INDEX(8,2)
      DO 2 J=1,5
    2 INDEX(J,1)=0
      I=0
    4 AMAX=-1.0
      DO 11 J=1,NP
      IF(INDEX(J,1)) 11,6,11
    6 DO 10 K=1,NP
      IF(INDEX(K,1)) 10,8,10
    8 P=DABS(A(J,K))
      IF(P.LE.AMAX) GO TO 10
      IR=J
      IC=K
      AMAX=P
   10 CONTINUE
   11 CONTINUE
      IF(AMAX) 30,30,14
   14 INDEX(IC,1)=IR
      IF(IR.EQ.IC) GO TO 18
      DO 16 L=1,NP
      P=A(IR,L)
      A(IR,L)=A(IC,L)
   16 A(IC,L)=P
      P=B(IR)
      B(IR)=B(IC)
      B(IC)=P
      I=I+1
      INDEX(I,2)=IC
   18 P=1./A(IC,IC)
      A(IC,IC)=1.0
      DO 20 L=1,NP
   20 A(IC,L)=A(IC,L)*P
      B(IC)=B(IC)*P
```

```
      DO 24 K=1,NP
      IF(K.EQ.IC) GO TO 24
      P=A(K,IC)
      A(K,IC)=0.0
      DO 22 L=1,NP
   22 A(K,L)=A(K,L)-A(IC,L)*P
      B(K)=B(K)-B(IC)*P
   24 CONTINUE
      GO TO 4
   26 IC=INDEX(I,2)
      IR=INDEX(IC,1)
      DO 28 K=1,NP
      P=A(K,IR)
      A(K,IR)=A(K,IC)
   28 A(K,IC)=P
      I=I-1
   30 IF(I) 26,32,26
   32 RETURN
      END
C
C     ------------
      SUBROUTINE MODELS(BB,YY,NOB,NCON,XX,M,PROD)
C
C     purpose: to calculate YY(X1,X2,X3,...)
C
      IMPLICIT REAL*8 (A-H,L,O-Z)
      LOGICAL PROD
      COMMON NPAR,CC,MODEL,NIV,INDEX
      COMMON/EVAL/ T,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,A,B,X1,X2,NGC
      PARAMETER(ZERO=0.0D+00,ZIP=1.0D-08,ONE=1.0D+00,TWO=2.0D+00,
     $FOUR=4.0D+00,EIGHT=8.0D+00)
      DIMENSION XX(4,NCON),YY(NCON),BB(16),CC(5),INDEX(8)
      EXTERNAL CF1,CT1,CF2,CT2,CF4,LAM2,LAM2C,CT4,LAM4,LAM4C,CF5,CT5,CS3
      PI=FOUR*DATAN(ONE)
C
      NGC=M
      K=0
      DO 5 I=9,NPAR
       IF (INDEX(I-8).EQ.0) GOTO 5
       K=K+1
       BB(I)=BB(K)
    5 CONTINUE
      V=BB(9)
      R=BB(10)
      TO=BB(11)
      RMU=BB(12)
      RLAM=BB(13)
      DX=BB(14)
      DY=BB(15)
      DZ=BB(16)
      CO=CC(1)
      A=CC(2)
      B=CC(3)
      X1=CC(4)
      X2=CC(5)
      DO 85 I=1,NOB
       T=XX(1,I)
       X=XX(2,I)
       Y=XX(3,I)
       Z=XX(4,I)
C
C     --- INLET AND INITIAL CONCENTRATIONS ---
       ZIP1=ABS(X-X1)
       ZIP2=ABS(X-X2)
       ZIPA=ABS(ABS(Y)-A)
```

```
      ZIPB=ABS(ABS(Z)-B)
      GOTO (25,25,35,35,45,45,55,55,65,65,25,35,55) MODEL
   25 IF (X.LT.ZIP .AND. MODEL.NE.2) THEN
       YY(I)=ZERO
       IF (Y.LT.0.0 .AND. Z.LT.0.0) YY(I)=CO
       IF ((ABS(Y).LT.ZIP .AND. Z.LT.0.0) .OR. (Y.LT.0.0
     $  .AND. ABS(Z).LT.ZIP)) YY(I)=CO/TWO
       IF (ABS(Y).LT.ZIP .AND. ABS(Z).LT.ZIP) YY(I)=CO/FOUR
       IF (MODEL.NE.11 .AND. T.GE.TO) YY(I)=ZERO
      ELSE IF (MODEL.NE.11 .AND. T.LT.ZIP) THEN
       YY(I)=ZERO
      ELSE
       GOTO 75
      ENDIF
      GOTO 85
C
   35 IF (X.LT.ZIP .AND. MODEL.NE.4) THEN
  YY(I)=ZERO
       IF (ABS(Y).LT.A .AND. ABS(Z).LT.B) YY(I)=CO
       IF ((ZIPA.LE.ZIP .AND. ABS(Z).LT.B) .OR. (ABS
     $  (Y).LT.A .AND. ZIPB.LE.ZIP)) YY(I)=CO/TWO
       IF (ZIPA.LE.ZIP .AND.ZIPB.LE.ZIP) YY(I)=CO/FOUR
       IF (MODEL.NE.12. AND. T.GE.TO) YY(I)=ZERO
      ELSE IF (MODEL.NE.12 .AND. T.LT.ZIP) THEN
       YY(I)=ZERO
      ELSE
       GOTO 75
      ENDIF
      GOTO 85
C
   45 IF (T.LT.ZIP) THEN
       IF (ZIP1.LE.ZIP .OR. ZIP2.LE.ZIP) THEN
        IF (ZIPA.LE.ZIP .AND. ZIPB.LE.ZIP) THEN
         YY(I)=CO/EIGHT
        ELSE IF ((ABS(Y).LT.A .AND. ZIPB.LE.ZIP) .OR. (ZIPA
     $   .LE.ZIP .AND. ABS(Z).LT.B)) THEN
         YY(I)=CO/FOUR
        ELSE IF (ABS(Y).LT.A .AND. ABS(Z).LT.B) THEN
         YY(I)=CO/TWO
        ELSE
         YY(I)=ZERO
        ENDIF
       ELSE IF (X.GT.X1 .AND. X.LT.X2) THEN
        IF (ZIPA.LE.ZIP .AND. ZIPB.LE.ZIP) THEN
         YY(I)=CO/FOUR
        ELSE IF (ZIPA.LE.ZIP .AND. ABS(Z).LT.B) THEN
         YY(I)=CO/TWO
        ELSE IF (ABS(Y).LT.A .AND. ZIPB.LE.ZIP) THEN
         YY(I)=CO/TWO
        ELSE IF (ABS(Y).LT.A .AND. ABS(Z).LT.B) THEN
         YY(I)=CO
        ELSE IF (ABS(Y).GT.A .OR. ABS(Z).GT.B) THEN
         YY(I)=ZERO
        ENDIF
       ELSE IF (X.LT.X1 .OR. X.GT.X2) THEN
        YY(I)=ZERO
       ENDIF
      ELSE
       GOTO 75
      ENDIF
      GOTO 85
C
  55  IF (X.LT.ZIP .AND. MODEL.NE.8) THEN
       YY(I)=ZERO
       IF (Y.LT.A) YY(I)=CO
```

```
      IF (ZIPA.LE.ZIP) YY(I)=CO/TWO
      IF (MODEL.NE.13 .AND. T.GE.TO) YY(I)=ZERO
     ELSE IF (T.LT.ZIP .AND. MODEL.NE.13) THEN
      YY(I)=ZERO
     ELSE
      GOTO 75
     ENDIF
     GOTO 85
C
   65 IF (T.LT.ZIP) THEN
      IF (ZIP1.LE.ZIP .OR. ZIP2.LE.ZIP) THEN
       IF (ZIPA.LE.ZIP) YY(I)=CO/FOUR
       IF (Y.LT.A) YY(I)=CO/TWO
       IF (Y.GT.A) YY(I)=ZERO
      ELSE IF (X.GT.X1 .AND. X.LT.X2) THEN
       IF (ZIPA.LE.ZIP) YY(I)=CO/TWO
       IF (Y.LT.A) YY(I)=CO
       IF (Y.GT.A) YY(I)=ZERO
      ELSE IF (X.LT.X1 .OR. X.GT.X2) THEN
       YY(I)=ZERO
      ENDIF
     ELSE
      GOTO 75
     ENDIF
     GOTO 85
C
   75 IF (MODEL.EQ.1) THEN
       CALL CHEBY(CF1,RES1,ZERO,T)
       IF(T.GT.TO) THEN
         PT=T-TO
         CALL CHEBY(CF1,RESP,ZERO,PT)
         RES1=RES1-RESP
       ENDIF
       IF (RLAM.GT.0. .AND. PROD)  CALL CHEBY(LAM2,RES2,ZERO,T)
       YY(I)=CO*RES1/FOUR+RLAM*RES2/TWO/R
     ELSE IF (MODEL.EQ.2) THEN
       CALL CHEBY(CT1,RES1,ZERO,T)
       IF(T.GT.TO) THEN
         PT=T-TO
         CALL CHEBY(CT1,RESP,ZERO,PT)
         RES1=RES1-RESP
       ENDIF
       IF (RLAM.GT.0..AND. PROD)  CALL CHEBY(LAM4,RES2,ZERO,T)
       YY(I)=CO*V*RES1/R/FOUR+RLAM*RES2/TWO/R
     ELSE IF (MODEL.EQ.3) THEN
       CALL CHEBY(CF2,RES1,ZERO,T)
       IF(T.GT.TO) THEN
         PT=T-TO
         CALL CHEBY(CF2,RESP,ZERO,PT)
         RES1=RES1-RESP
       ENDIF
       IF (RLAM.GT.0. .AND. PROD)  CALL CHEBY(LAM2,RES2,ZERO,T)
       YY(I)=CO*RES1/FOUR+RLAM*RES2/TWO/R
     ELSE IF (MODEL.EQ.4) THEN
       CALL CHEBY(CT2,RES1,ZERO,T)
       IF(T.GT.TO) THEN
         PT=T-TO
         CALL CHEBY(CT2,RESP,ZERO,PT)
         RES1=RES1-RESP
       ENDIF
       IF (RLAM.GT.0. .AND. PROD)  CALL CHEBY(LAM4,RES2,ZERO,T)
       YY(I)=CO*V*RES1/R/FOUR+RLAM*RES2/TWO/R
     ELSE IF (MODEL.EQ.5) THEN
       IF (RLAM.GT.0. .AND. PROD)  CALL CHEBY(LAM2,RES2,ZERO,T)
       YY(I)=CO*LAM5(T)*GAMMA2(T)/EIGHT+RLAM*RES2/TWO/R
```

```
      ELSE IF (MODEL.EQ.6) THEN
        IF (RLAM.GT.0. .AND. PROD)  CALL CHEBY(LAM4,RES2,ZERO,T)
        Y1=CO*LAM6(T)*GAMMA2(T)/EIGHT
        Y2=RLAM*RES2/TWO/R
        YY(I)=y1+y2
      ELSE IF (MODEL.EQ.7) THEN
        CALL CHEBY(CF4,RES1,ZERO,T)
        IF(T.GT.TO) THEN
          PT=T-TO
          CALL CHEBY(CF4,RESP,ZERO,PT)
          RES1=RES1-RESP
        ENDIF
        IF (RLAM.GT.0. .AND. PROD)  CALL CHEBY(LAM2,RES2,ZERO,T)
        YY(I)=CO*RES1/TWO+RLAM*RES2/TWO/R
      ELSE IF (MODEL.EQ.8) THEN
        CALL CHEBY(CT4,RES1,ZERO,T)
        IF(T.GT.TO) THEN
          PT=T-TO
          CALL CHEBY(CT4,RESP,ZERO,PT)
          RES1=RES1-RESP
        ENDIF
        IF (RLAM.GT.0..AND. PROD) CALL CHEBY(LAM4,RES2,ZERO,T)
        YY(I)=CO*RES1*V/TWO/R+RLAM*RES2/TWO/R
      ELSE IF (MODEL.EQ.9) THEN
        CALL CHEBY(CF5,RES1,ZERO,A)
        IF (RLAM.GT.0. .AND. PROD) CALL CHEBY(LAM2,RES2,ZERO,T)
        YY(I)=CO*RES1/FOUR+RLAM*RES2/TWO/R
      ELSE IF (MODEL.EQ.10) THEN
        CALL CHEBY(CT5,RES1,ZERO,A)
        IF (RLAM.GT.0..AND. PROD) CALL CHEBY(LAM4,RES2,ZERO,T)
        YY(I)=CO*RES1/FOUR+RLAM*RES2/TWO/R
      ELSE IF (MODEL.EQ.11) THEN
        YY(I)=CO*EXF(ZERO,Y/DSQRT(FOUR*DY*X/V))
     $      *EXF(ZERO,Z/DSQRT(FOUR*DZ*X/V))/FOUR
      ELSE IF (MODEL.EQ.12) THEN
        YY(I)=CO/FOUR*(EXF(ZERO,(Y-A)/DSQRT(FOUR*DY*X/V))
     $       -EXF(ZERO,(Y+A)/DSQRT(FOUR*DY*X/V)))
     $       *(EXF(ZERO,(Z-B)/DSQRT(FOUR*DZ*X/V))
     $       -EXF(ZERO,(Z+B)/DSQRT(FOUR*DZ*X/V)))
      ELSE IF (MODEL.EQ.13) THEN
        CALL CHEBY(CS3,RES,ZERO,A)
        YY(I)=CO*RES
      ENDIF
C
   85 CONTINUE
C
      RETURN
      END
C
C     ----------
      REAL*8 FUNCTION CF1(T)
      IMPLICIT REAL*8(A-M,O-Z)
      COMMON/EVAL/TT,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,A,B,X1,X2,NGC
      PARAMETER(ZERO=0.0D+00,ZIP=1.0D-08,FOUR=4.0D+00)
      PI=4.0D+00*DATAN(1.0D+00)
C
      IF(T.LE.ZIP) T=ZIP
      CF1=(X/T)*DSQRT(R/(FOUR*PI*DX*T))
     $ *DEXP(-RMU*T/R-(R*X-V*T)**2/FOUR/R/DX/T)
     $ *EXF(ZERO,Y/DSQRT(FOUR*DY*T/R))*EXF(ZERO,Z/DSQRT(FOUR*DZ*T/R))
C
      RETURN
      END
C
C     ----------
```

```
      REAL*8 FUNCTION CT1(T)
      IMPLICIT REAL*8(A-M,O-Z)
      COMMON/EVAL/TT,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,A,B,X1,X2,NGC
      PARAMETER(ZERO=0.0D+00,ZIP=1.0D-08,TWO=2.0D+00,FOUR=4.0D+00)
      PI=4.0D+00*DATAN(1.0D+00)
C
      IF(T.LE.ZIP) T=ZIP
      CT1=(DSQRT(R/PI/DX/T)*DEXP(-RMU*T/R-(R*X-V*T)**2/FOUR/R/DX/T)
     $   -V/TWO/DX*EXF(V*X/DX-RMU*T/R,(R*X+V*T)/DSQRT(FOUR*R*DX*T)))
     $   *EXF(ZERO,Y/DSQRT(FOUR*DY*T/R))*EXF(ZERO,Z/DSQRT(FOUR*DZ*T/R))
C
      RETURN
      END
C
C     ----------
      REAL*8 FUNCTION CF2(T)
      IMPLICIT REAL*8(A-M,O-Z)
      COMMON/EVAL/TT,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,A,B,X1,X2,NGC
      PARAMETER(ZERO=0.0D+00,ZIP=1.0D-08,FOUR=4.0D+00)
      PI=4.0D+00*DATAN(1.0D+00)
C
      IF(T.LE.ZIP) T=ZIP
      CF2=(X/T)*DSQRT(R/(FOUR*PI*DX*T))
     $    *DEXP(-RMU*T/R-(R*X-V*T)**2/FOUR/R/DX/T)
     $    *(EXF(ZERO,(Y-A)/DSQRT(FOUR*DY*T/R))
     $    -EXF(ZERO,(Y+A)/DSQRT(FOUR*DY*T/R)))
     $    *(EXF(ZERO,(Z-B)/DSQRT(FOUR*DZ*T/R))
     $    -EXF(ZERO,(Z+B)/DSQRT(FOUR*DZ*T/R)))
C
      RETURN
      END
C
C     ----------
      REAL*8 FUNCTION CT2(T)
      IMPLICIT REAL*8(A-M,O-Z)
      COMMON/EVAL/TT,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,A,B,X1,X2,NGC
      PARAMETER(ZERO=0.0D+00,ZIP=1.0D-08,TWO=2.0D+00,FOUR=4.0D+00)
      PI=4.0D+00*DATAN(1.0D+00)
C
      IF(T.LE.ZIP) T=ZIP
      CT2=(DSQRT(R/PI/DX/T)*DEXP(-RMU*T/R-(R*X-V*T)**2/FOUR/R/DX/T)
     $    -V/TWO/DX*EXF(V*X/DX-RMU*T/R,(R*X+V*T)/DSQRT(FOUR*R*DX*T)))
     $    *(EXF(ZERO,(Y-A)/DSQRT(FOUR*DY*T/R))
     $    -EXF(ZERO,(Y+A)/DSQRT(FOUR*DY*T/R)))
     $    *(EXF(ZERO,(Z-B)/DSQRT(FOUR*DZ*T/R))
     $    -EXF(ZERO,(Z+B)/DSQRT(FOUR*DZ*T/R)))
C
      RETURN
      END
C
C     ----------
      REAL*8 FUNCTION CF4(T)
      IMPLICIT REAL*8(A-M,O-Z)
      COMMON/EVAL/TT,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,A,B,X1,X2,NGC
      PARAMETER(ZERO=0.0D+00,FOUR=4.0D+00)
      EXTERNAL CF41
      PI=4.0D+00*DATAN(1.0D+00)
C
      CALL CHEONE(CF41,T,RES,ZERO,A)
      CF4=RES
      RETURN
      END
C
C     ----------
      REAL*8 FUNCTION CF41(RHO,T)
```

```
      IMPLICIT REAL*8(A-M,O-Z)
      COMMON/EVAL/TT,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,A,B,X1,X2,NGC
      PARAMETER(ZERO=0.0D+00,ZIP=1.0D-08,TWO=2.0D+00,FOUR=4.0D+00)
      PI=4.0D+00*DATAN(1.0D+00)
C
      IF(T.LE.ZIP) T=ZIP
      CF41=(X/T)*DSQRT(R/(FOUR*PI*DX*T))
     $     *DEXP(-RMU*T/R-(R*X-V*T)**2/FOUR/R/DX/T)
     $     *RHO*R/DY/T*EXPBI0(R*Y*RHO/TWO/DY/T,
     $     -(R*(Y**2+RHO**2)/FOUR/DY/T))
C
      RETURN
      END
C
C     ----------
      REAL*8 FUNCTION CT4(T)
      IMPLICIT REAL*8(A-M,O-Z)
      COMMON/EVAL/TT,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,A,B,X1,X2,NGC
      PARAMETER(ZERO=0.0D+00,FOUR=4.0D+00)
      EXTERNAL CT41
      PI=4.0D+00*DATAN(1.0D+00)
C
      CALL CHEONE(CT41,T,RES,ZERO,A)
      CT4=RES
      RETURN
      END
C
C     ----------
      REAL*8 FUNCTION CT41(RHO,T)
      IMPLICIT REAL*8(A-M,O-Z)
      COMMON/EVAL/TT,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,A,B,X1,X2,NGC
      PARAMETER(ZERO=0.0D+00,ZIP=1.0D-08,TWO=2.0D+00,FOUR=4.0D+00)
      PI=4.0D+00*DATAN(1.0D+00)
C
      IF(T.LE.ZIP) T=ZIP
      CT41=(DSQRT(R/PI/DX/T)*DEXP(-RMU*T/R-(R*X-V*T)**2/FOUR/R/DX/T)
     $      -V/TWO/DX*EXF(V*X/DX-RMU*T/R,(R*X+V*T)/DSQRT(FOUR*R*DX*T)))
     $      *RHO*R/DY/T*EXPBI0(R*Y*RHO/TWO/DY/T,
     $      -(R*(Y**2+RHO**2)/FOUR/DY/T))
C
      RETURN
      END
C
C     ----------
      REAL*8 FUNCTION CF5(RHO)
      IMPLICIT REAL*8(A-M,O-Z)
      COMMON/EVAL/ T,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,A,B,X1,X2,NGC
      PARAMETER(ZERO=0.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
      PI=4.0D+00*DATAN(1.0D+00)
      CF5=(EXF(-RMU*T/R,(R*(X-X2)-V*T)/DSQRT(FOUR*R*DX*T))
     $     -EXF(-RMU*T/R,(R*(X-X1)-V*T)/DSQRT(FOUR*R*DX*T))
     $     +EXF(V*X/DX-RMU*T/R,(R*(X+X2)+V*T)/DSQRT(FOUR*R*DX*T))
     $     -EXF(V*X/DX-RMU*T/R,(R*(X+X1)+V*T)/DSQRT(FOUR*R*DX*T)))
     $     *RHO*R/DY/T*EXPBI0(R*Y*RHO/TWO/DY/T,
     $     -(R*(Y**2+RHO**2)/FOUR/DY/T))
C
      RETURN
      END
C
C     ----------
      REAL*8 FUNCTION CT5(RHO)
      IMPLICIT REAL*8(A-M,O-Z)
      COMMON/EVAL/ T,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,A,B,X1,X2,NGC
      PARAMETER(ZERO=0.0D+00,ONE=1.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
      PI=4.0D+00*DATAN(1.0D+00)
```

```
      CT5=CO/FOUR*((ONE+V/DX*(X+X1)+V**2*T/R/DX)
     $       *EXF(V*X/DX-RMU*T/R,(R*(X+X1)+V*T)/DSQRT(FOUR*R*DX*T))
     $       -(ONE+V/DX*(X+X2)+V**2*T/R/DX)
     $       *EXF(V*X/DX-RMU*T/R,(R*(X+X2)+V*T)/DSQRT(FOUR*R*DX*T))
     $       +EXF(-RMU*T/R,(R*(X-X2)-V*T)/DSQRT(FOUR*R*DX*T))
     $       -EXF(-RMU*T/R,(R*(X-X1)-V*T)/DSQRT(FOUR*R*DX*T))
     $       +DSQRT(FOUR*V**2*T/PI/R/DX)
     $       *(DEXP(V*X/DX-RMU*T/R-(R*(X+X2)+V*T)**2/FOUR/R/DX/T)
     $       -DEXP(V*X/DX-RMU*T/R-(R*(X+X1)+V*T)**2/FOUR/R/DX/T)))
     $       *RHO*R/DY/T*EXPBIO(R*Y*RHO/TWO/DY/T,
     $       -(R*(Y**2+RHO**2)/FOUR/DY/T))
C
      RETURN
      END
C
C     ----------
      REAL*8 FUNCTION CS3(RHO)
      IMPLICIT REAL*8(A-M,O-Z)
      COMMON/EVAL/ T,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,A,B,X1,X2,NGC
      PARAMETER(ZERO=0.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
C
      CS3=RHO*V/DY/X/TWO*EXPBIO(V*Y*RHO/TWO/DY/X,
     $   -(V*(Y**2+RHO**2)/FOUR/DY/X))
C
      RETURN
      END
C
C     ----------
      REAL*8 FUNCTION GAMMA2(T)
      IMPLICIT REAL*8(A-M,O-Z)
      COMMON/EVAL/TT,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,A,B,X1,X2,NGC
      PARAMETER(ZERO=0.0D+00,FOUR=4.0D+00)
C
      GAMMA2=(EXF(ZERO,(Y-A)/DSQRT(FOUR*DY*T/R))
     $        -EXF(ZERO,(Y+A)/DSQRT(FOUR*DY*T/R)))
     $        *(EXF(ZERO,(Z-B)/DSQRT(FOUR*DZ*T/R))
     $        -EXF(ZERO,(Z+B)/DSQRT(FOUR*DZ*T/R)))
      RETURN
      END
C
C     ----------
      REAL*8 FUNCTION LAM2(T)
      IMPLICIT REAL*8(A-M,O-Z)
      COMMON/EVAL/TT,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,A,B,X1,X2,NGC
      PARAMETER(ZERO=0.0D+00,ZIP=1.0D-08,FOUR=4.0D+00)
      PI=4.0D+00*DATAN(1.0D+00)
C
      LAM2=EXF(-RMU*T/R,(V*T-R*X)/DSQRT(FOUR*R*DX*T))
     $       -EXF(V*X/DX-RMU*T/R,(R*X+V*T)/DSQRT(FOUR*R*DX*T))
      RETURN
      END
C
C     ----------
      REAL*8 FUNCTION LAM4(T)
      IMPLICIT REAL*8(A-M,O-Z)
      COMMON/EVAL/TT,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,A,B,X1,X2,NGC
      PARAMETER(ZERO=0.0D+00,ONE=1.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
      PI=4.0D+00*DATAN(1.0D+00)
C
      LAM4=EXF(-RMU*T/R,(V*T-R*X)/DSQRT(FOUR*R*DX*T))+
     $      (ONE+V*X/DX+V**2*T/R/DX)*EXF(V*X/DX-RMU*T/R,(R*X+V*T)/
     $      DSQRT(FOUR*R*DX*T))-DSQRT(FOUR*V**2*T/PI/R/DX)*
     $      DEXP(-RMU*T/R-(R*X-V*T)**2/FOUR/R/DX/T)
      RETURN
      END
```

```
C
C     ----------
      REAL*8 FUNCTION LAM5(T)
      IMPLICIT REAL*8(A-M,O-Z)
      COMMON/EVAL/TT,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,A,B,X1,X2,NGC
      PARAMETER(FOUR=4.0D+00)
C
      LAM5=EXF(-RMU*T/R,(R*(X-X2)-V*T)/DSQRT(FOUR*R*DX*T))
     $    -EXF(-RMU*T/R,(R*(X-X1)-V*T)/DSQRT(FOUR*R*DX*T))
     $    +EXF(V*X/DX-RMU*T/R,(R*(X+X2)+V*T)/DSQRT(FOUR*R*DX*T))
     $    -EXF(V*X/DX-RMU*T/R,(R*(X+X1)+V*T)/DSQRT(FOUR*R*DX*T))
      RETURN
      END
C
C     ----------
      REAL*8 FUNCTION LAM6(T)
      IMPLICIT REAL*8(A-M,O-Z)
      COMMON/EVAL/TT,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,A,B,X1,X2,NGC
      PARAMETER(ZERO=0.0D+00,ONE=1.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
      PI=4.0D+00*DATAN(1.0D+00)
C
      LAM6=(ONE+V/DX*(X+X1)+V**2*T/R/DX)
     $     *EXF(V*X/DX-RMU*T/R,(R*(X+X1)+V*T)/DSQRT(FOUR*R*DX*T))
     $     -(ONE+V/DX*(X+X2)+V**2*T/R/DX)
     $     *EXF(V*X/DX-RMU*T/R,(R*(X+X2)+V*T)/DSQRT(FOUR*R*DX*T))
     $     +EXF(-RMU*T/R,(R*(X-X2)-V*T)/DSQRT(FOUR*R*DX*T))
     $     -EXF(-RMU*T/R,(R*(X-X1)-V*T)/DSQRT(FOUR*R*DX*T))
     $     +DSQRT(FOUR*V**2*T/PI/R/DX)
     $     *(DEXP(V*X/DX-RMU*T/R-(R*(X+X2)+V*T)**2/FOUR/R/DX/T)
     $     -DEXP(V*X/DX-RMU*T/R-(R*(X+X1)+V*T)**2/FOUR/R/DX/T))
      RETURN
      END
C
C     --------------
      FUNCTION EXF(A,B)
C
C     PURPOSE:  TO CALCULATE EXP(A) ERFC(B)
C
      IMPLICIT REAL*8(A-M,O-Z)
      EXF=0.D00
      IF((DABS(A).GT.100.).AND.(B.LE.0.)) RETURN
      C=A-B*B
      IF((DABS(C).GT.100.).AND.(B.GE.0.)) RETURN
      IF(C.LT.-100.) GO TO 3
      X=DABS(B)
      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 EXF=Y*DEXP(C)
    3 IF(B.LT.0.0) EXF=2.*DEXP(A)-EXF
C
      RETURN
      END
C
C     ----------
      REAL*8 FUNCTION EXPBIO(X,Z)
      IMPLICIT REAL*8(A-M,O-Z)
C
C     PURPOSE: TO CALCULATE EXP(Z)*Io(X) FOR ANY REAL X AND Z
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/
      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
      IF (DABS(X).LT.3.75) THEN
       Y=(X/3.75)**2
       EXPBI0=DEXP(Z)*(P1+Y*(P2+Y*(P3+Y*(P4+Y*(P5+Y*(P6+Y*P7))))))
      ELSE
       AX=DABS(X)
       Y=3.75/AX
       EXPBI0=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   ----------------------------------------------
      SUBROUTINE CHEBY(FUNC,AREA,A,B)
C
C     PURPOSE: PERFORM INTEGRATION OF F(X) BETWEEN A AND B
C              USING M-POINT GAUSS-CHEBYSHEV QUADRATURE FORMULA
      IMPLICIT REAL*8 (A-M,O-Z)
      COMMON/EVAL/ T,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,AA,BB,X1,X2,NGC
      PARAMETER(ZERO=0.0D+00,ONE=1.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
      PI=FOUR*DATAN(ONE)
      AREA=ZERO
      SUM=ZERO
      DO 10 I=1,NGC
        Z1=DCOS(DFLOAT(2*(I-1)+1)*PI/DFLOAT(2*NGC))
        TAU=(Z1*(B-A)+B+A)/TWO
   10 SUM=SUM+FUNC(TAU)*DSQRT(ONE-Z1*Z1)
      AREA=(B-A)*PI*SUM/DFLOAT(2*NGC)
C
      RETURN
      END
C
C   ----------------------------------------------
      SUBROUTINE CHEONE(FUNC,T,AREA,A,B)
C
C     PURPOSE: PERFORM FIRST INTEGRATION OF F(X,T) BETWEEN A AND B
C              USING M-POINT GAUSS-CHEBYSHEV QUADRATURE FORMULA
      IMPLICIT REAL*8 (A-M,O-Z)
      COMMON/EVAL/TT,X,Y,Z,V,R,TO,RMU,RLAM,DX,DY,DZ,CO,AA,BB,X1,X2,NGC
      PARAMETER(ZERO=0.0D+00,ONE=1.0D+00,TWO=2.0D+00,FOUR=4.0D+00)
      PI=FOUR*DATAN(ONE)
      AREA=ZERO
      SUM=ZERO
      DO 10 I=1,NGC
        Z1=DCOS(DFLOAT(2*(I-1)+1)*PI/DFLOAT(2*NGC))
        RHO=(Z1*(B-A)+B+A)/TWO
   10 SUM=SUM+FUNC(RHO,T)*DSQRT(ONE-Z1*Z1)
      AREA=(B-A)*PI*SUM/DFLOAT(2*NGC)
C
      RETURN
      END
```