MODIFICATION OF A METHOD-OF-CHARACTERISTICS SOLUTE-TRANSPORT MODEL TO INCORPORATE DECAY AND EQUILIBRIUM-CONTROLLED SORPTION OR ION EXCHANGE

By Daniel J. Goode and Leonard F. Konikow

U.S. GEOLOGICAL SURVEY

Water-Resources Investigations Report 89-4030

Reston, Virginia
1989

DEPARTMENT OF THE INTERIOR

MANUEL LUJAN, JR., Secretary

U.S. GEOLOGICAL SURVEY

Dallas L. Peck, Director

For additional information
write to:

Project Chief
U.S. Geological Survey
431 National Center
Reston, Virginia 22092

Copies of this report can
be purchased from:

U.S. Geological Survey
Books and Open-File Reports Section
Federal Center, Building 41
Box 25425
Denver, Colorado 80225

CONTENTS

ILLUSTRATIONS

TABLES

CONVERSION FACTORS

For use of readers who prefer to use inch-pound units, conversion factors for the metric (International System) units used in this report are listed below:

Multiply metric units	by	To Obtain Inch-Pound Units
centimeter (cm)	0.03281	foot (ft)
meter (m)	3.281	foot (ft)
centimeter squared per second (cm^2/s)	0.001076	foot squared per second (ft^2/s)
meter squared per day (m^2/d)	10.76	foot squared per day (ft^2/d)
milligram (mg)	2.205×10^{-6}	pound (lb)
liter (L)	0.03531	cubic foot (ft^3)
mole per liter (mol/L)	28.32	mole per cubic foot (mol/ft^3)

PREFACE

This report presents modifications to a digital computer model for calculating changes in the concentration of dissolved chemical species in flowing ground water. The computer program represents a basic and general model that may have to be modified by the user for efficient application to his specific field problem. Although this model will produce reliable calculations for a wide variety of field problems, the user is cautioned that in some cases the accuracy and efficiency of the model can be affected significantly by the discretization and the selection of values for certain other user-specified options.

The user is requested to notify the originating office of any errors found in this report or in the computer program. Updates may occasionally be made to both the report and the computer program. Users who wish to be added to the mailing list to receive updates, if any, may send a request to the originating office at the following address:

U.S. Geological Survey
431 National Center
Reston, VA 22092

Copies of the computer program on tape or disk are available at cost of processing from:

U.S. Geological Survey
WATSTORE Program Office
437 National Center
Reston, VA 22092
Telephone: 703/648-5695

MODIFICATION OF A METHOD-OF-CHARACTERISTICS SOLUTE-TRANSPORT MODEL TO INCORPORATE DECAY AND EQUILIBRIUM-CONTROLLED SORPTION OR ION EXCHANGE

By Daniel J. Goode and Leonard F. Konikow

ABSTRACT

The U.S. Geological Survey computer model of two-dimensional solute transport and dispersion in ground water (Konikow and Bredehoeft, 1978) has been modified to incorporate the following types of chemical reactions: (1) first-order irreversible rate-reaction, such as radioactive decay; (2) reversible equilibrium-controlled sorption with linear, Freundlich, or Langmuir isotherms; and (3) reversible equilibrium-controlled ion exchange for monovalent or divalent ions. Numerical procedures are developed to incorporate these processes in the general solution scheme that uses method-of-characteristics with particle tracking for advection and finite-difference methods for dispersion. The first type of reaction is accounted for by an exponential decay term applied directly to the particle concentration. The second and third types of reactions are incorporated through a retardation factor, which is a function of concentration for nonlinear cases. The model is evaluated and verified by comparison with analytical solutions for linear sorption and decay, and by comparison with other numerical solutions for nonlinear sorption and ion exchange.

(p. 3 follows)

INTRODUCTION

Konikow and Bredehoeft (1978) developed a general computer model of two-dimensional transport and dispersion in ground water for conservative (non-reactive) solutes. Recent experience, particularly with contamination problems, indicates the need to account for the effects of various chemical reactions on transport. The purpose of this report is to present modifications of the model of Konikow and Bredehoeft that incorporate a first-order, irreversible rate-reaction, linear and nonlinear equilibrium-controlled sorption, and equilibrium-controlled ion exchange. An example of a first-order, irreversible rate-reaction is radioactive decay. The reversible, equilibrium reactions considered are linear sorption, Freundlich sorption, Langmuir sorption, monovalent ion exchange, divalent ion exchange, monovalent-divalent ion exchange, and divalent-monovalent ion exchange. The reversible equilibrium assumption allows formulation of a single advection-dispersion equation with a retardation factor that accounts for the chemical reaction. The assumption of instantaneous and reversible equilibrium may be appropriate for many solute-transport problems, but the validity of this assumption should be evaluated independently for each application.

This report presents the mathematical development of these chemical reaction terms and describes the numerical procedures incorporating these terms in the general transport model. The algorithms for the nonlinear retardation factor are essentially those developed by Grove and Stollenwerk (1984). Model results are compared to analytical solutions and to results from the model of Grove and Stollenwerk (1984) for one-dimensional problems. Two-dimensional results are also presented and compared to results from the SUTRA (Saturated Unsaturated TRAnsport) model (Voss, 1984) and to an analytical solution. The appendixes include changes to the computer program, input and output for an example problem, and input formats.

The solution of the ground-water flow equation is not affected by these modifications, hence this report considers only transport. This report should be used in conjunction with the model's original documentation (Konikow and Bredehoeft, 1978) and subsequent updates (see Preface).

The contributions of Mark Person to early development of numerical algorithms and code verification are gratefully acknowledged.

THEORY

General Transport Equation

The governing equation for the solute-transport model considers flow and transport in two dimensions and assumes constant and uniform porosity and fluid density. The general governing equation for solute transport is (after Konikow and Grove, 1977)

$$\frac{\partial C}{\partial t} = \frac{1}{b}\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right) - V_i\frac{\partial C}{\partial x_i} + \frac{W(C-C')}{\varepsilon b} + \frac{CHEM}{\varepsilon} , \qquad (1)$$

where	C	is the concentration of the solute, ML^{-3};
	t	is time, T;
	b	is the aquifer thickness, L;
	D_{ij}	is the dispersion tensor, L^2T^{-1}, with implied summation for i=1,2, j=1,2;
	x_i	are the spatial coordinates, L;
	V_i	is the fluid seepage velocity, LT^{-1};
	W	is the source fluid flux into ($W<0$) the aquifer, LT^{-1};
	ε	is the porosity, (dimensionless);
	C'	is the concentration of the solute in the source fluid, ML^{-3}; and
	CHEM	is the chemical reaction source (+) or sink (-) per unit volume of aquifer, $ML^{-3}T^{-1}$.

The dispersion, advection, and fluid source terms in (1) are discussed in detail by Konikow and Grove (1977) and Konikow and Bredehoeft (1978) and will not be addressed further here.

In this work, the reaction term CHEM includes equilibrium-controlled sorption or exchange and first-order irreversible rate (decay) reactions. The general expression for the chemical reaction source or sink is (Grove and Stollenwerk, 1984)

$$CHEM = -\rho_b\frac{d\bar{C}}{dt} - \lambda(\varepsilon C+\rho_b\bar{C}) , \qquad (2)$$

where	$\bar{C}$	is the concentration of solute sorbed (or exchanged) on the porous medium, MM^{-1};

ρ_b is the porous medium bulk density, ML^{-3}; and
λ is the decay rate constant, T^{-1}.

Substituting eq. 2 into the general governing equation (eq. 1), and rearranging results in

$$\frac{\partial C}{\partial t} + \frac{\rho_b}{\varepsilon}\frac{d\overline{C}}{dt} = \frac{1}{b}\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right) - V_i\frac{\partial C}{\partial x_i} + \frac{W(C-C')}{\varepsilon b} - \lambda C - \frac{\rho_b}{\varepsilon}\lambda\overline{C} \ . \qquad (3)$$

Decay

The decay term (second term on right hand side of eq. 2) commonly represents radioactive decay, but it can also represent chemical decomposition or biodegradation. First-order production occurs if $\lambda<0$. Radioactive decay rates are often expressed as half-lives ($t_{1/2}$), where the half-life is the time required for the concentration to decrease to one-half of the original value:

$$t_{1/2} = \frac{(\ln 2)}{\lambda} \ . \qquad (4)$$

The form of eq. 3 is only valid if the solute in solution and that sorbed decay at the same rate. This assumption is true for radioactive decay but may not be appropriate for chemical decomposition or biodegradation.

Linear Sorption

The temporal change in sorbed concentration in eq. 3 can be represented in terms of the solute concentration using the chain rule of calculus, as follows:

$$\frac{d\overline{C}}{dt} = \frac{d\overline{C}}{dC}\frac{\partial C}{\partial t} \ . \qquad (5)$$

For equilibrium sorption and exchange reactions $d\overline{C}/dC$, as well as $\overline{C}$, is a function of C alone. Therefore, the equilibrium relation for $\overline{C}$ and $d\overline{C}/dC$ can be substituted into the governing equation to develop a partial differential equation in terms of C only. The resulting single transport equation is solved for solute concentration. Sorbed concentration can then be calculated using the equilibrium relation. In the case of ion exchange, concentrations of the second exchanging ion, as well as the exchange site concentrations of both ions, can be determined from the concentration of one of the ions.

The linear-sorption exchange reaction considers that the concentration of solute sorbed to the porous medium is directly proportional to the concentration of the solute in the pore fluid, according to the relation

$$\bar{C} = K_d C \ , \tag{6}$$

where K_d is the distribution coefficient, L^3M^{-1}. This reaction is assumed to be instantaneous and reversible. The slope (derivative) of the sorbed concentration versus dissolved concentration curve, $d\bar{C}/dC$, is simply the equilibrium distribution coefficient, K_d.

Using eq. 6 and the chain rule (eq. 5),

$$\frac{d\bar{C}}{dt} = \frac{d\bar{C}}{dC}\frac{\partial C}{\partial t} = K_d\frac{\partial C}{\partial t} \ ; \tag{7}$$

then, eq. 3 becomes

$$\frac{\partial C}{\partial t} + \frac{\rho_b K_d}{\varepsilon}\frac{\partial C}{\partial t} = \frac{1}{b}\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right) - V_i\frac{\partial C}{\partial x_i} + \frac{W(C-C')}{\varepsilon b} - \lambda C - \frac{\rho_b K_d}{\varepsilon}\lambda C \ . \tag{8}$$

Factoring out the term $(1 + \rho_b K_d/\varepsilon)$ and defining a retardation factor, R_f (dimensionless), as:

$$R_f = 1 + \frac{\rho_b K_d}{\varepsilon} \ , \tag{9}$$

results in

$$R_f \frac{\partial C}{\partial t} = \frac{1}{b} \frac{\partial}{\partial x_i}\left(bD_{ij} \frac{\partial C}{\partial x_j} \right) - V_i \frac{\partial C}{\partial x_i} + \frac{W(C-C')}{\varepsilon b} - R_f \lambda C \ . \qquad (10)$$

Because R_f is constant under these assumptions, the solution to this governing equation is identical to the solution to the governing equation with no sorption effects, except that the velocity, dispersion coefficient, and source strength are reduced by a factor R_f. The transport process thus appears to be "retarded" because of the instantaneous equilibrium sorption onto the porous medium.

Nonlinear Sorption

For nonlinear sorption, the slope $d\overline{C}/dC$ is not constant, but depends on the solute concentration. Figure 1 shows sorbed concentration as a function of solute concentration for a linear isotherm ($K_d = 1$), a Freundlich isotherm, and a Langmuir isotherm. The parameters for the nonlinear isotherms are identified below. Although $d\overline{C}/dC$ is not constant, for any given concentration a linearized R_f can be determined that will apply to the movement of solute at that concentration. Thus, in the governing equation (eq. 10) the constant R_f on the left-hand side can be replaced by a function, $R_f(C)$:

$$R_f(C) = 1 + \frac{\rho_b}{\varepsilon} \frac{d\overline{C}}{dC} \ . \qquad (11)$$

This formulation assumes that C and $d\overline{C}/dC$ are continuous in space; it is not appropriate for discontinuous or "shock" fronts (Charbeneau, 1981). The R_f on the right-hand side of eq. 10 accounts for decay of sorbed mass (see eq. 3) and can be replaced by the term $1 + \rho_b \overline{C}/(\varepsilon C)$.

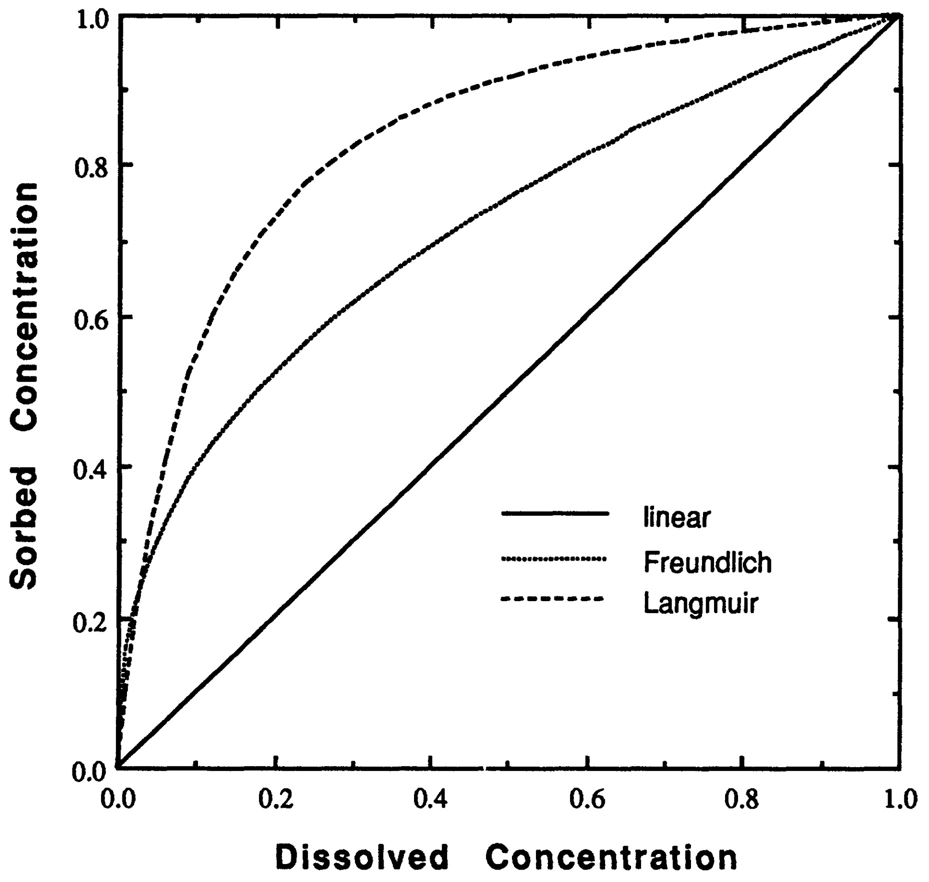

Figure 1. Sorbed concentration as a function of solute concentration for linear, Freundlich, and Langmuir isotherms.

Substitution of the nonlinear retardation factor (eq. 11) and the irreversible rate-reaction into eq. 3 to incorporate decay and nonlinear sorption or ion-exchange results in

$$\frac{\partial C}{\partial t} = \frac{1}{bR_f(C)}\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{V_i}{R_f(C)}\frac{\partial C}{\partial x_i} + \frac{W(C-C')}{\varepsilon bR_f(C)} - \frac{\lambda}{R_f(C)}\left(C + \frac{\rho_b}{\varepsilon}\bar{C}\right), \quad (12)$$

where $R_f(C)$ and $\bar{C}$ are defined below for linear sorption, Freundlich sorption, Langmuir sorption, and four cases of ion exchange with monovalent or divalent ions. For the case of linear sorption, the last term in eq. 12 reduces to $-\lambda C$ and $R_f(C) = R_f$ is constant.

Freundlich Sorption

The Freundlich sorption isotherm is

$$\bar{C} = K_f C^n \ , \tag{13}$$

where K_f is the Freundlich sorption equilibrium constant (units are a function of n); and

n is the Freundlich exponent, (dimensionless).

The slope of the nonlinear isotherm is

$$\frac{d\bar{C}}{dC} = n \, K_f \, C^{n-1} \ . \tag{14}$$

This slope is constant and equal to K_f if $n = 1$ (that is, the isotherm is linear). The retardation factor is

$$R_f(C) = 1 + \frac{\rho_b}{\varepsilon} n \, K_f \, C^{n-1} \ . \tag{15}$$

In figure 1, the parameters for the Freundlich isotherm are $K_f = 1$ and $n = 0.7$.

Langmuir Sorption

The Langmuir equilibrium sorption isotherm considers a porous medium with a maximum available sorption capacity, according to the relation

$$\bar{C} = \frac{K_\ell Q C}{(1 + K_\ell C)} \ , \tag{16}$$

where K_ℓ is the Langmuir sorption equilibrium constant, L^3M^{-1}; and

Q is the maximum sorption capacity, MM^{-1}.

The slope of this isotherm is

$$\frac{d\bar{C}}{dC} = \frac{K_\ell Q C}{(1 + K_\ell C)^2} \ . \qquad (17)$$

At low concentrations, the slope approaches $K_\ell Q$, a constant. At high concentrations, the slope approaches zero, as the medium will not sorb additional solute. The corresponding retardation factor is

$$R_f(C) = 1 + \frac{\rho_b}{\varepsilon}\left[\frac{K_\ell Q C}{(1 + K_\ell C)^2}\right] \ . \qquad (18)$$

In figure 1, the parameters for the Langmuir isotherm are $K_\ell = 10$ and $Q = 1.1$.

Ion Exchange

The ion-exchange processes under consideration follow mass-action equilibrium for the relation

$$mC_1^n + n\bar{C}_2 \leftrightarrow m\bar{C}_1 + nC_2^m \ , \qquad (19)$$

where n is the valence for ion 1;
m is the valence for ion 2; and
$\bar{C}$ is the exchange-site concentration.

For ion-exchange problems, useful concentration units are moles or equivalents per volume, rather than units of mass per volume.

The ion-exchange selectivity coefficient, K_m (dimensionless), for this reaction is (Freeze and Cherry, 1979)

$$K_m = \frac{[\bar{C}_1]^m \, [C_2]^n}{[\bar{C}_2]^n \, [C_1]^m} \ . \qquad (20)$$

The total-solution concentration (the sum of the equivalence concentrations of the two competing ions in solution) and the ion-exchange capacity are assumed to be constant so that the concentration of ion 2 can be expressed in terms of ion 1 concentrations (Grove and Stollenwerk, 1984), as follows:

$$C_2 = (C_0 - nC_1)/m \quad ; \qquad \bar{C}_2 = (Q - n\bar{C}_1)/m \ , \tag{21}$$

where C_0 is the total-solution concentration, ML^{-3}; and
Q is the ion-exchange capacity, MM^{-1}.

The ion-exchange capacity is analogous to the maximum sorption capacity for the Langmuir sorption isotherm and the same symbol, Q, is used for both. For a specific transport problem, only one of these processes would be simulated. Substituting these expressions (eq. 21) into eq. 20 yields the selectivity coefficient in terms of ion 1 alone, as follows:

$$K_m = \frac{[\bar{C}]^m \left[\frac{C_0 - nC}{m}\right]^n}{[C]^m \left[\frac{Q - n\bar{C}}{m}\right]^n} \ , \tag{22}$$

where the subscripts on C_1 and $\bar{C}_1$ have been dropped. Eq. 22 can be rearranged to express the exchanged concentration $\bar{C}$ as a function of the solution concentration C and several constants. Furthermore, $d\bar{C}/dC$ can be determined and substituted into eq. 11 for the nonlinear retardation factor.

The slope of the ion-exchange relationship for C is a function of the ion valences as well as C_0, K_m, and Q. The linearized retardation factors are presented for four cases (Grove and Stollenwerk, 1984):

(1) monovalent-monovalent--for example, exchange of sodium (C), n=1, and potassium, m=1:

$$R_f(C) = 1 + \frac{\rho_b}{\varepsilon}\left(\frac{K_m Q C_0}{[C(K_m - 1) + C_0]^2}\right) ; \tag{23}$$

(2) divalent-divalent--for example, exchange of calcium (C), n=2, and strontium, m=2:

$$R_f(C) = 1 + \frac{\rho_b}{\varepsilon}\left(\frac{K_m Q C_0}{[2C(K_m-1) + C_0]^2}\right) ; \tag{24}$$

(3) monovalent-divalent--for example, exchange of sodium (C), n=1, and calcium, m=2:

$$R_f(C) = 1 + \frac{\rho_b}{\varepsilon}\left[\frac{\bar{C}^2 - 2\bar{C}CK_m + 2CK_mQ}{2\bar{C}(C_0-C) + C^2K_m}\right] , \tag{25a}$$

where $\bar{C}$, the exchange-site sodium concentration in eq. 25a, is given by the positive root of the quadratic equation

$$\bar{C}^2(C_0-C) + \bar{C}(K_mC^2) - K_mQC^2 = 0 ; \tag{25b}$$

(4) divalent-monovalent--for example, exchange of calcium (C), n=2, and sodium, m=1:

$$R_f(C) = 1 + \frac{\rho_b}{\varepsilon}\left[\frac{4K_m\bar{C}(Q-\bar{C}) - 4\bar{C}(C_0-2C) - K_mQ^2}{-4K_mC(Q-2\bar{C}) - (C_0-2C)^2}\right] , \tag{26a}$$

where $\bar{C}$, the exchange-site calcium concentration in eq. 26a, is given by the positive root of the quadratic equation

$$\bar{C}^2(4K_mC) + \bar{C}\left[-4K_mQC-(C_0-2C)^2\right] + K_mQ^2C = 0 . \tag{26b}$$

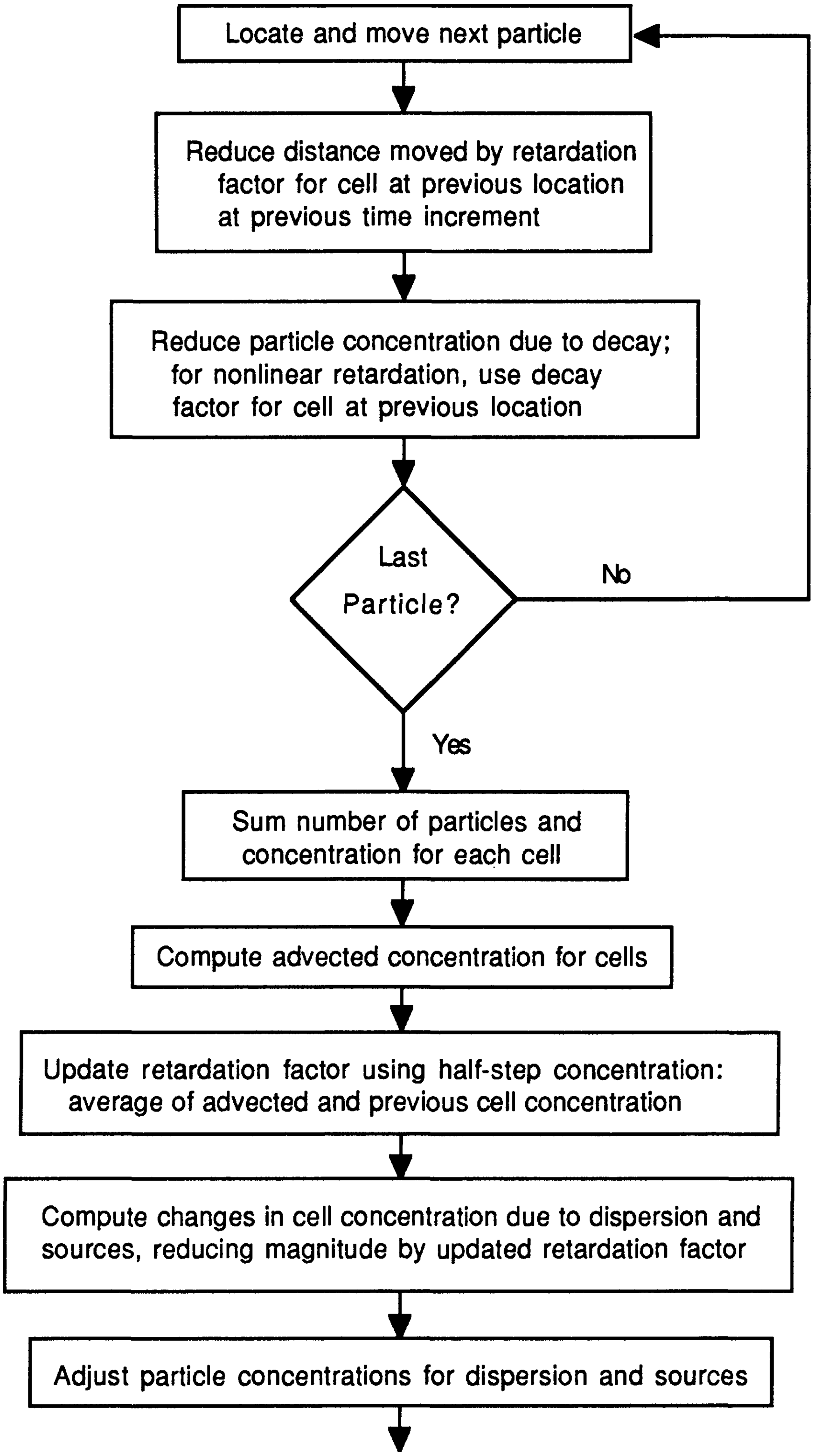

Figure 2. Flow chart showing major steps in transport simulation.

The time-step size for the numerical solution of the transport equation is determined from the numerical stability criteria and from parameter CELDIS, which limits particle movement to a specified fraction of the cell (grid) dimensions. Each of these criteria requires the maximum advective velocity, which is a function of retardation. For linear sorption, the retardation factor is constant and known *a priori*, and the maximum apparent or retarded velocity value can be calculated directly. For nonlinear sorption or ion exchange, the retardation factor is a function of concentration. The maximum concentration from either the initial condition or from the sources is used to compute a minimum retardation factor. This minimum retardation factor is then used with the maximum flow velocity value to determine the time-step size for particle moves. For one special case, Freundlich sorption with exponent (n) greater than 1, the minimum retardation is determined from the minimum concentration (internal parameter CZERO). The minimum retardation factor is recomputed for each pumping period.

Nonlinear Freundlich and Langmuir sorption processes have been incorporated into a version of this model modified previously (Tracy, 1982). In that work, the velocity values (which are computed at cell boundaries; see Konikow and Bredehoeft (1978)) were divided by the retardation factor, and these velocity values were then used for particle advection and used to compute the dispersion coefficients at cell boundaries. This approach possesses two problems. First, because retardation factors are based on cell concentrations, an average retardation factor must be determined for the boundaries between cells where velocity is calculated. This averaging smooths the retardation factors and results in different retardation factors for each particle and for the dispersion terms. The retardation factor represents sorbed storage and a unique value, corresponding to the concentration, should be used. The current approach avoids this problem by reducing the particle velocity by the retardation factor for the cell where the particle is located at the beginning of the time step.

The second problem is that the approach of Tracy (1982) causes the retardation factor to be brought within the derivative for the dispersion term because the dispersion coefficients are computed from the retarded velocities. The governing equation is then

$$\frac{\partial C}{\partial t} = \frac{1}{b}\frac{\partial}{\partial x_i}\left(\frac{bD_{ij}}{R_f(C)}\frac{\partial C}{\partial x_j}\right) + \text{remaining terms} \;, \qquad (31)$$

instead of the correct governing equation (see eq. 12)

NUMERICAL METHODS AND COMPUTER PROGRAM

Decay

The first-order, irreversible rate-reaction is solved using an exponential function to change directly the concentration of each particle. The change in concentration resulting only from decay can be isolated from eq. 3 as

$$\left(1 + \frac{\rho_b}{\varepsilon}\frac{d\bar{C}}{dC}\right)\frac{\partial C}{\partial t} = -\lambda\left(C + \frac{\rho_b}{\varepsilon}\bar{C}\right) , \qquad (27)$$

or

$$\frac{\partial C}{\partial t} = -\lambda C\left(\frac{1 + \frac{\rho_b}{\varepsilon}\frac{\bar{C}}{C}}{1 + \frac{\rho_b}{\varepsilon}\frac{d\bar{C}}{dC}}\right) . \qquad (28)$$

For the case of linear sorption, $\bar{C}/C = K_d$ and $d\bar{C}/dC = K_d$ so that the parenthetical term in eq. 28 has a value of 1. The denominator of the parenthetical term is, of course, the retardation factor, $R_f(C)$. The analytical solution to eq. 28 for the case of linear sorption yields the new particle concentration in the presence of decay, as follows:

$$C_{(t+\Delta t)} = C_{(t)} \exp(-\lambda\Delta t) \ . \qquad (29)$$

This representation is exact for problems with decay only, irrespective of time-step size (Δt).

For cases of nonlinear sorption or ion exchange, $\bar{C}/C \neq d\bar{C}/dC$, and both are not constant, therefore eq. 28 cannot be solved exactly. An approximation for decay in the nonlinear case is

$$C_{(t+\Delta t)} = C_{(t)} \exp\left[-\lambda \Delta t \left(\frac{1 + \frac{\rho_b}{\varepsilon} \frac{\bar{C}}{C}}{R_f\,(C)} \right) \right] , \qquad (30)$$

where the bracketed exponential term is evaluated for $C_{(t)}$. The retardation factor is developed using the chain rule and the slope (derivative) of the sorption isotherm, whereas the decay term acts on the actual mass sorbed and does not include the slope of the isotherm. This exponential formulation has no numerical stability restrictions. However, if the half-life is on the order of the time step or smaller, then accuracy will be lost because of the explicit decoupling of decay and other transport processes. In addition, eq. 30 is a linearized approximation and accuracy will be lost if the ratio in the exponential term changes significantly during the time step.

Retardation Factor

The solute-transport model uses a method-of-characteristics solution for the advection term in the governing solute-transport equation, whereas the dispersion and source terms are solved using explicit finite-difference methods (Konikow and Bredehoeft, 1978). Retardation is incorporated into the particle-tracking and dispersion calculations explicitly. As each particle is moved along a characteristic curve, its velocity is retarded using a linearized retardation factor computed explicitly for each time step using the cell concentration from the previous time step. Then changes in concentration resulting from dispersion are calculated. The retardation factor for dispersion and source calculations is computed from the half-step cell concentration, which is the average of the cell concentration at the end of the previous time step and the new cell concentration after accounting for advection and decay only. The use of an explicit retardation factor for these calculations is consistent with the existing explicit calculation for sources and dispersion using half-step cell concentrations and the explicit decoupling of advection and dispersion (Konikow and Bredehoeft, 1978). Although the algorithms do not add any new stability requirements, it is recognized that the time-step size may strongly affect model results if sorption or exchange is highly nonlinear over the simulated concentration range. Figure 2 illustrates the major steps during solution of the transport problem with retardation.

$$\frac{\partial C}{\partial t} = \frac{1}{bR_f(C)}\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right) + \text{remaining terms} \ . \qquad (32)$$

The retardation factor accounts for accretion (storage) in the sorbed phase and must remain outside all spatial derivatives, analogous to the porosity term. The current approach reduces dispersive flux for each cell using only the retardation factor for that cell, consistent with the governing equation (eq. 12). Tracy's approach will yield significant errors only if $R_f(C)$ changes significantly from cell to cell. For linear sorption, the retardation factor is constant and the two approaches yield identical results.

An alternative approach to using the cell concentration to compute nonlinear retardation factors is to compute retardation factors for each particle based on that particle's concentration. However, adjacent particles on the same streamline or pathline may have significantly different concentrations because of the model's computational procedures. In this approach, because the retarded velocities could be very different, particles on the same pathline could move past one another. In reality, local physical mixing would provide a unique concentration and associated retardation effect at each location; parcels of water having one concentration do not move past (through) downgradient parcels having another concentration. Therefore, retardation factors are best computed using the cell concentration, which averages all of the particle concentrations within a cell. Even with this approach, particles may pass each other when time steps are very large because of the use of explicit velocities (see discussion of model parameter CELDIS by Konikow and Bredehoeft (1978)). If the basic particle and cell averaging of the model resulted in particle concentrations reflecting the local mixing, then it would possibly be more accurate to compute the retardations from the individual particle concentrations. However, such modifications to the basic numerical procedures are beyond the scope of the present work.

The development of explicit retardation factors for the nonlinear cases is only appropriate for smooth or continuous fronts. This is because the change in sorbed storage as a sharp front moves is not equal to the slope of the sorption isotherm, which is discontinuous at a sharp front (Charbeneau, 1981). Therefore, this model should not be used for cases having both nonlinear sorption (or ion exchange) and no dispersion. For similar reasons, large errors in the rate of front movement may occur if the retardation factor changes significantly between adjacent cells.

Implementation

Linear retardation and decay computations are inserted into existing subroutines (Appendix A). The calculation of nonlinear retardation factors and sorbed concentrations are performed by two new subprograms: SUBROUTINE RETRD2 - retardation functions; and FUNCTION SORB2 - sorbed concentrations. A third FUNCTION subprogram, QUADX, solves the quadratic equation needed for unequal valence ion-exchange calculations. These algorithms are based on those presented by Grove and Stollenwerk (1984). A common block /CHMR/ is added to store coefficients for decay and retardation calculations. Arrays for cell retardation factors are added in common block /CHMR2/. Appendix A documents the changes to the computer program showing statements to be deleted and added. These changes are applied to the version of the model as previously updated in November, 1988.

Input formats are compatible with previous versions of the model and are described in Appendix D. Equilibrium reaction types, including linear sorption, are selected using IREACT, in columns 69-72 on input card 2. If IREACT>0, then card 3.1 must be inserted after card 3. The values of IREACT corresponding to different reactions and the parameters on input card 3.1 are shown in Appendix D.

The type of reaction selected and input parameter values are printed on the output. Sorbed mass is also included in the mass balance calculations although the values of sorbed concentration corresponding to the calculated solute distribution are not printed.

EVALUATION OF MODEL RESULTS

One-dimensional Transport with Linear Sorption and Decay

Numerous analytical solutions are available for solute transport with linear sorption and radioactive decay. For one-dimensional transport in uniform flow in the x-direction the applicable governing equation is

$$R_f \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} - R_f \lambda C \ . \tag{33}$$

Boundary conditions include specified constant concentration at the origin--that is,

$$C=1 \quad \text{at } x = 0, \ \ t > 0 \ , \tag{34a}$$

and advection alone (no dispersion) at the end of the domain, as given by

$$\frac{\partial^2 C}{\partial x^2} = 0 \quad \text{at } x = L \ , \tag{34b}$$

where L = 100 centimeters (cm) is the length of the domain. The numerical results are compared to the analytical solutions (Van Genuchten and Alves, 1982) for this system for various combinations of parameters (V = 25 centimeters per day (cm/d) and D = 37.5 centimeters squared per day (cm^2/d) for all cases). As can be seen in figure 3, the agreement is excellent for all cases.

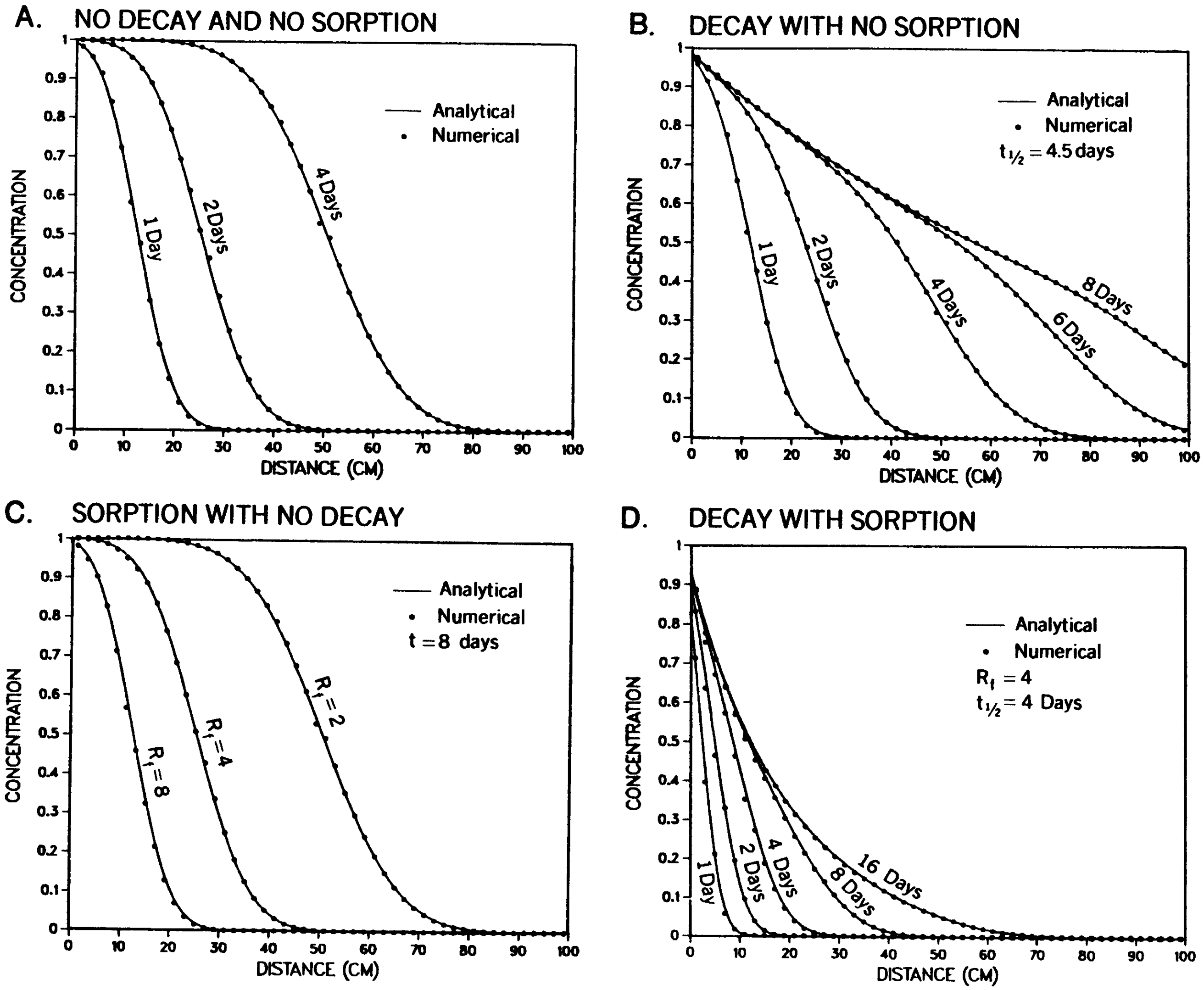

Figure 3. Comparison of numerical and analytical solutions for transport with reaction in one-dimensional, steady flow (Δx = 2 centimeters, V = 25 centimeters per day, and D = 37.5 centimeters squared per day in all cases): (A) no decay and no sorption; (B) decay with no sorption, (C) sorption with no decay, (D) decay with sorption.

One-dimensional Transport with Nonlinear Sorption and Exchange

General analytical solutions to the solute-transport problem with nonlinear equilibrium sorption and ion exchange are not available. Therefore, it is not possible to verify the model calculations by comparison with analytical solutions. However, the retardation factors are essentially constant for certain values of the sorption isotherm and ion-exchange parameters. At these limiting values, the results for each separate chemical process can be compared to the analytical solution for linear (constant) retardation. In addition, the model results can be compared to other numerical models for cases with nonlinear retardation.

The model results are compared to the results using the one-dimensional finite-difference model of Grove and Stollenwerk (1984). A flux boundary condition has been used for both models, and for the limiting linear analytical solution. The governing equation for these examples is (Grove and Stollenwerk, 1984)

$$R_f(C)\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x} - \lambda\left(C + \frac{\rho_b}{\varepsilon}\bar{C}\right) . \qquad (35)$$

A flux boundary condition at $x = 0$ is imposed as follows:

$$(C_I - C)V = -D\frac{\partial C}{\partial x} \qquad \text{at } x = 0 \ , \qquad (36a)$$

where C_I is the solute concentration in the added water; and a semi-infinite boundary condition at $x = +\infty$ is imposed as follows:

$$C = 0 \qquad \text{at } x = +\infty \ . \qquad (36b)$$

The numerical-model boundary condition at $x = L = 16$ cm is advective flux only, $\partial^2 C/\partial x^2 = 0$, which approximates the boundary condition for the analytical solution (eq. 36b).

The retardation factor, R_f, is a constant for the linear case, and is a function of C for the nonlinear reactions. For constant R_f, and no decay ($\lambda = 0$), the analytical solution to this problem is (Van Genuchten and Alves, 1982; Bear, 1979; Gershon and Nir, 1969):

$$\frac{C}{C_I} = \frac{1}{2}\operatorname{erfc}\left[\frac{R_f x - Vt}{(4R_f Dt)^{1/2}}\right] - \frac{1}{2}\exp\left(\frac{Vx}{D}\right)\operatorname{erfc}\left[\frac{R_f x + Vt}{(4R_f Dt)^{1/2}}\right]\left[1 + V\left(\frac{R_f x + Vt}{R_f D}\right)\right]$$

$$+ V\left[\frac{t}{\pi R_f D}\right]^{1/2}\exp\left[\frac{Vx}{D} - \frac{(R_f x + Vt)^2}{4R_f Dt}\right], \qquad (37)$$

where erfc is the complementary error function. (Note: the last exponential term contains typographical errors in the latter two references.) The parameter values are shown in table 1.

Table 1. -- Parameters for one-dimensional nonlinear examples

Uniform velocity in x-direction	$V = 0.1$ cm/s
Dispersion coefficient	$D = 0.01$ cm^2/s
Porosity	$\varepsilon = 0.37$
Bulk density of porous medium	$\rho_b = 1.587$ g/ml
Duration of source pulse	80 s
Source concentration	$C_I = 0.05$ and 5 E-5 mol/L
Linear sorption equilibrium coefficient	$K_d = 0.3$ ml/g
Freundlich equilibrium coefficient	$K_f = 0.3$ (units vary)
Freundlich slope exponent	$n = 0.7$ and 1.0
Langmuir equilibrium coefficient	$K_\ell = 100$ ml/g
Maximum sorption capacity	$Q = 0.003$ eqv/g
Total solution concentration	$C_0 = 0.1$ eqv/L
Ion-exchange equilibrium coefficients	
Monovalent-monovalent	$K_m = 10$
Divalent-divalent	$K_m = 10$
Monovalent-divalent	$K_m = 3$
Divalent-monovalent	$K_m = 333$
Decay half-life	
Freundlich case	$t_{1/2} = 693.15$ s
Langmuir case	$t_{1/2} = 69.315$ s

A 12-cm column is discretized by 120 cells. The CELDIS parameter, which controls time-step size for the transport simulation, is set at 0.25 and the initial particle density is NPTPND = 16. The model of Grove and Stollenwerk (1984) is applied with a 16-cm column discretized by 100 finite-difference nodes and with a time-step criterion of CDELT = 0.2. These simulations are similar to those presented by Grove and Stollenwerk (1984), except that a smaller dispersion coefficient is used, the source pulse duration is halved, and a flux boundary condition is used. Figures 4 to 10 show the time history of solute concentration at 8 cm versus pore volumes for the present model, the model of Grove and Stollenwerk (1984), and for the analytical solution (eq. 37) with the corresponding limiting value of constant retardation. Pore volume is a dimensionless variable proportional to time, equal to Vt/x. Figure 4 shows the cases of no reactions and linear sorption (constant retardation).

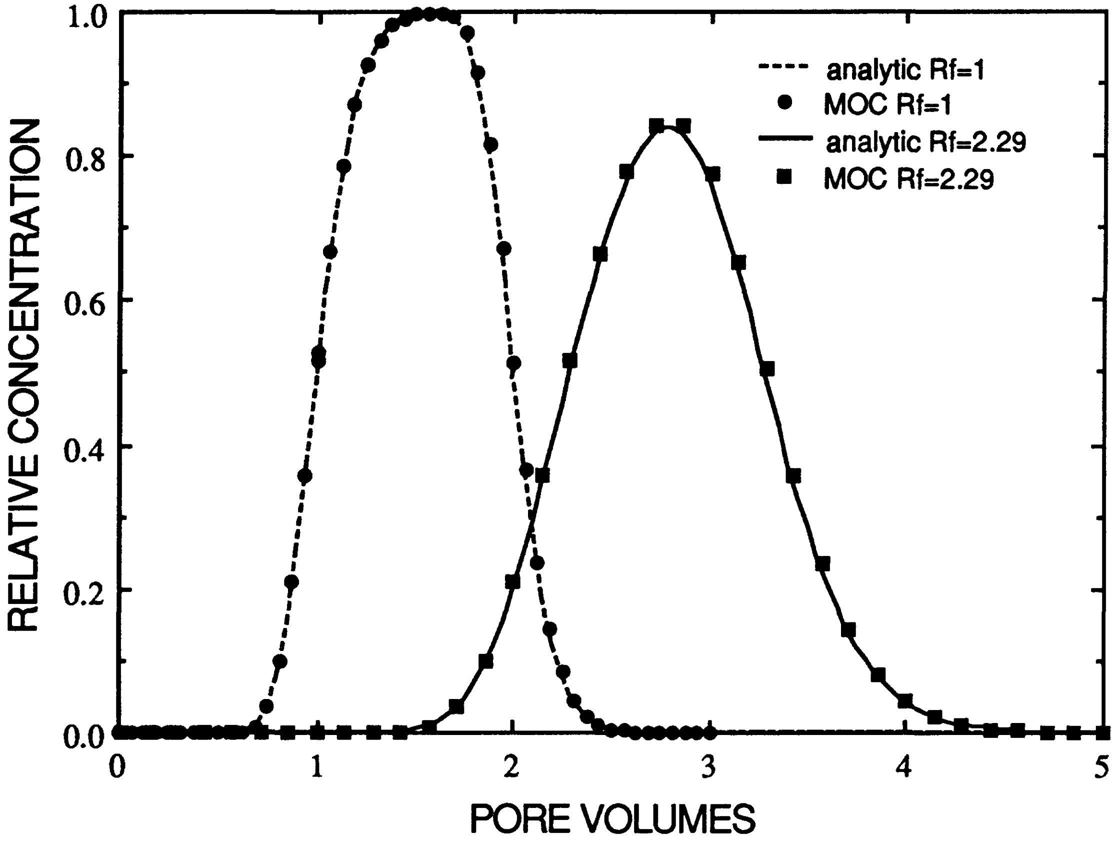

Figure 4. Breakthrough for transport in one-dimensional flow with no reactions and with linear sorption ("MOC" is the present work).

Figures 5 and 6 illustrate Freundlich and Langmuir sorption, respectively. The Freundlich isotherm with exponent n=1 is equivalent to linear sorption and, as shown, the model results agree with the analytical solution for linear sorption. With a nonlinear Freundlich isotherm (n=0.7), the pulse is retarded more and breakthrough occurs later. However, because solute mass is more strongly sorbed at lower concentrations, the breakthrough curve is still steep. Under the assumption of linear sorption, increased retardation also produces greater spreading (in time) as shown in figure 4, which is distinct from the nonlinear effect (fig. 5). Incorporation of decay further reduces concentrations, most noticeably at the peak. The relative nonlinearity of the Langmuir isotherms is changed by changing the input concentrations (fig. 6). For low input concentrations, the Langmuir isotherm is essentially linear, and the model results agree with the analytical solution for linear sorption. For higher input concentrations, the isotherm is nonlinear and a lower fraction of solute mass is sorbed. Thus, breakthrough occurs earlier (fig. 6). The nonlinear nature of the isotherm produces the sharp breakthrough and distinctive long tailing. The present results agree with those using the model of Grove and Stollenwerk (1984).

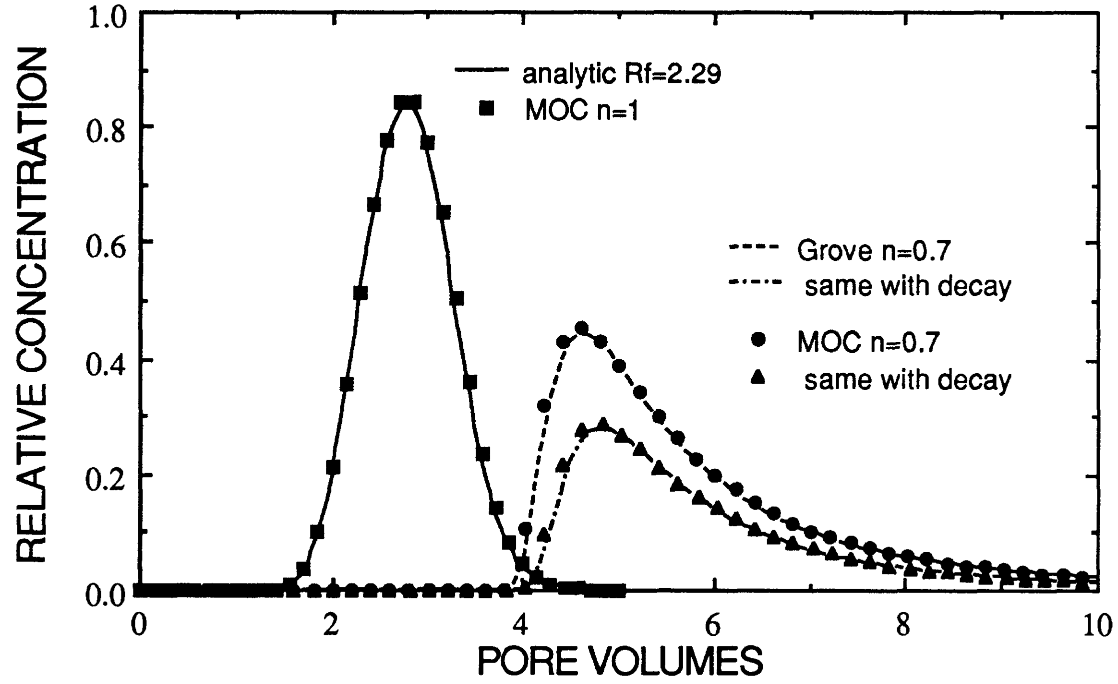

Figure 5. Breakthrough for transport in one-dimensional flow with Freundlich sorption ("Grove" is the model of Grove and Stollenwerk (1984), "MOC" is the present work).

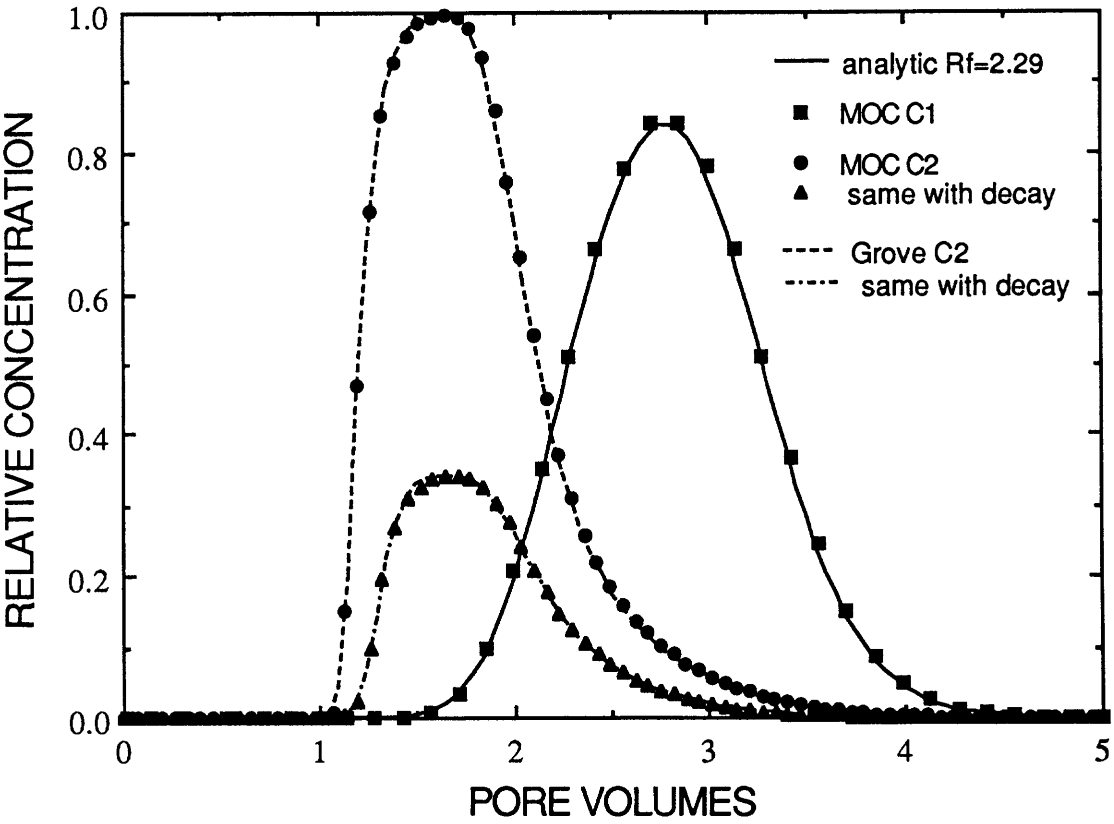

Figure 6. Breakthrough for transport in one-dimensional flow with Langmuir sorption ("Grove" is the model of Grove and Stollenwerk (1984), "MOC" is the present work, C1 = input concentration of 0.00005 milligrams per liter, C2 = input concentration of 0.05 milligrams per liter).

Figures 7, 8, 9, and 10 show model results for the cases of monovalent-monovalent ion exchange, divalent-divalent ion exchange, monovalent-divalent ion exchange, and divalent-monovalent ion exchange, respectively. The breakthrough curves for the ion-exchange examples are similar to those for the Langmuir isotherm. Again, at low input concentrations, the exchange process is essentially linear, and results agree with the analytical solution with linear sorption. At higher input concentrations, a lower fraction of solute mass is exchanged, and breakthrough occurs earlier. The nonlinear nature of the ion-exchange process yields a steep breakthrough curve with tailing.

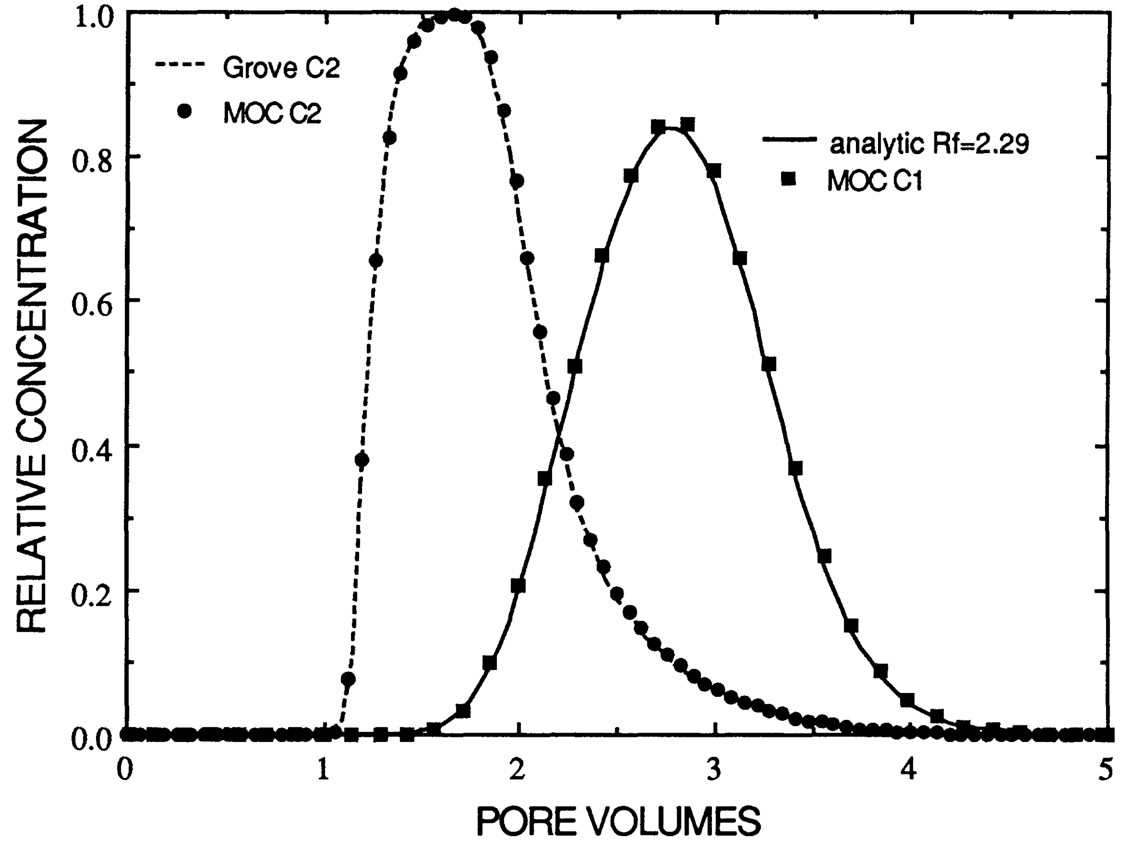

Figure 7. Breakthrough for transport in one-dimensional flow with monovalent-monovalent ion exchange ("Grove" is the model of Grove and Stollenwerk (1984), "MOC" is the present work, C1 = input concentration of 0.00005 milligrams per liter, C2 = input concentration of 0.05 milligrams per liter).

Reasonable agreement with the results using the model of Grove and Stollenwerk (1984) is demonstrated for all cases. The case of Freundlich sorption (fig. 5), which is the most nonlinear of those presented, shows the poorest agreement, as expected. The nonlinear nature of the sorption and exchange processes results in the extended tails in the plots; at lower concentrations, the retardation factor is higher.

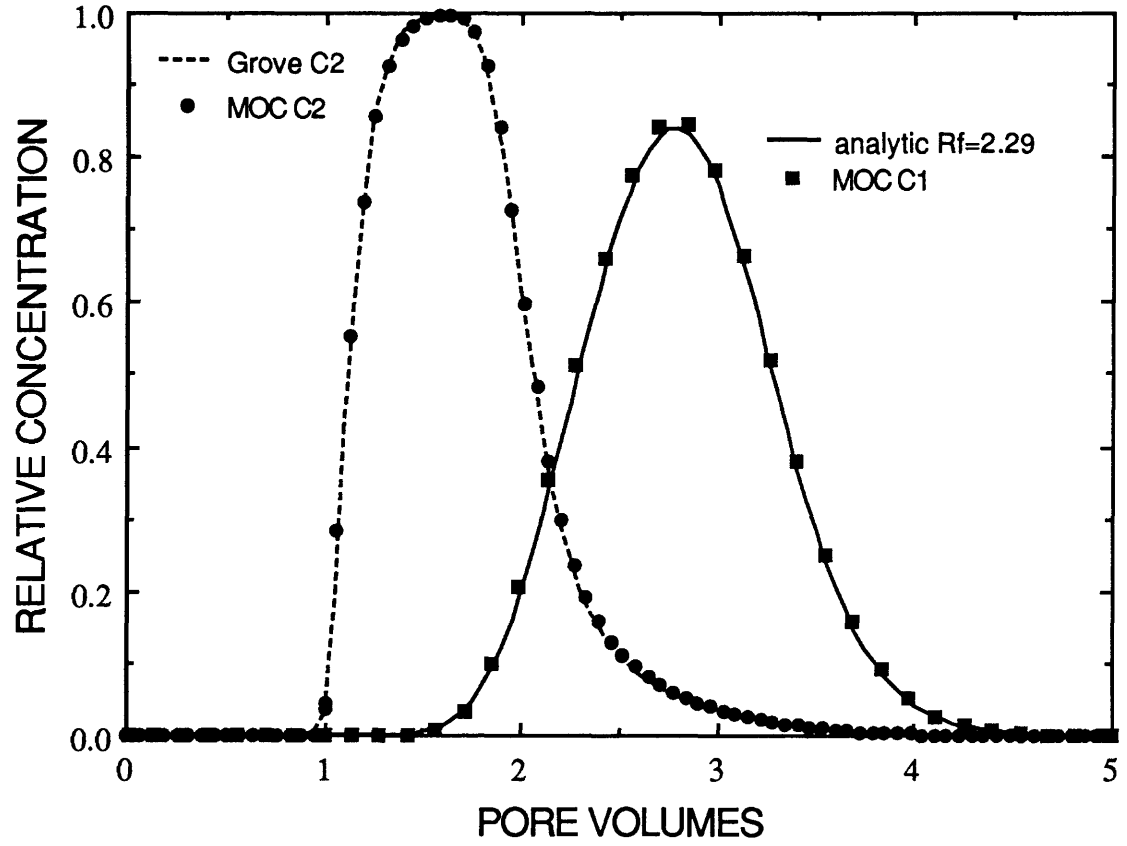

Figure 8. Breakthrough for transport in one-dimensional flow with divalent-divalent ion exchange ("Grove" is the model of Grove and Stollenwerk (1984), "MOC" is the present work, C1 = input concentration of 0.00005 milligrams per liter, C2 = input concentration of 0.05 milligrams per liter).

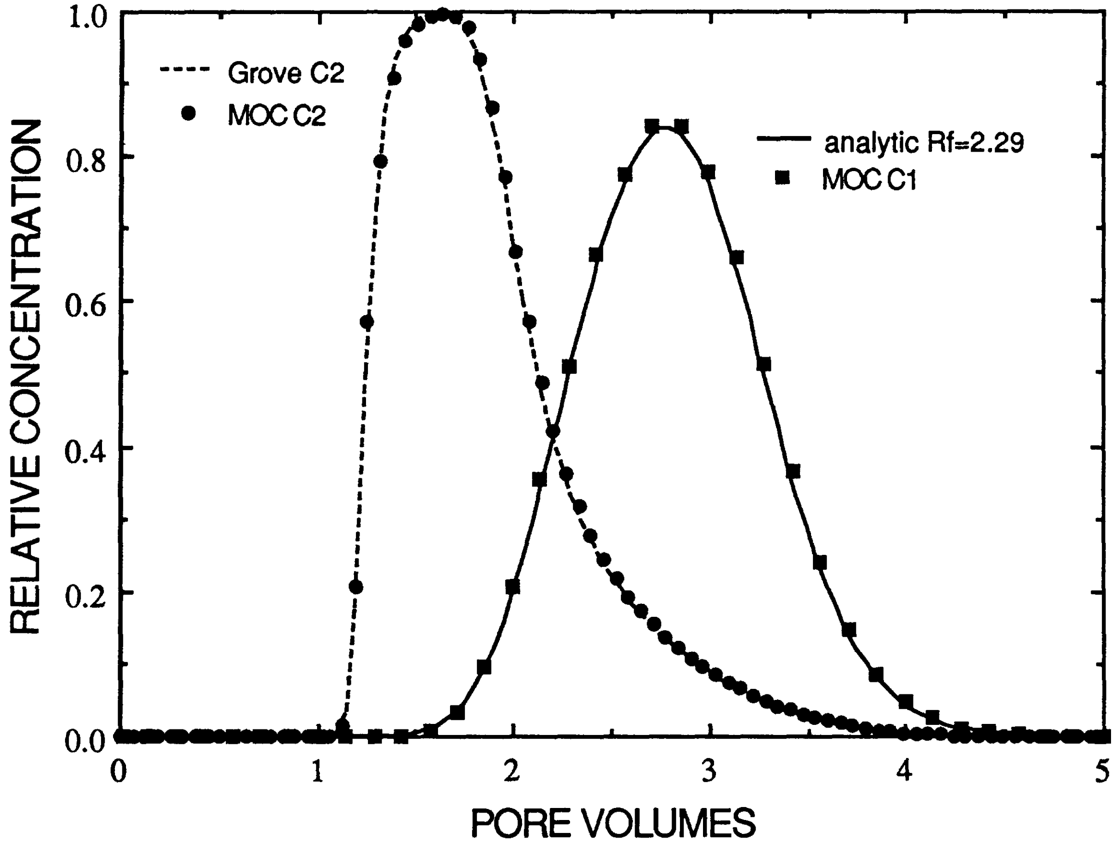

Figure 9. Breakthrough for transport in one-dimensional flow with monovalent-divalent ion exchange ("Grove" is the model of Grove and Stollenwerk (1984), "MOC" is the present work, C1 = input concentration of 0.00005 milligrams per liter, C2 = input concentration of 0.05 milligrams per liter).

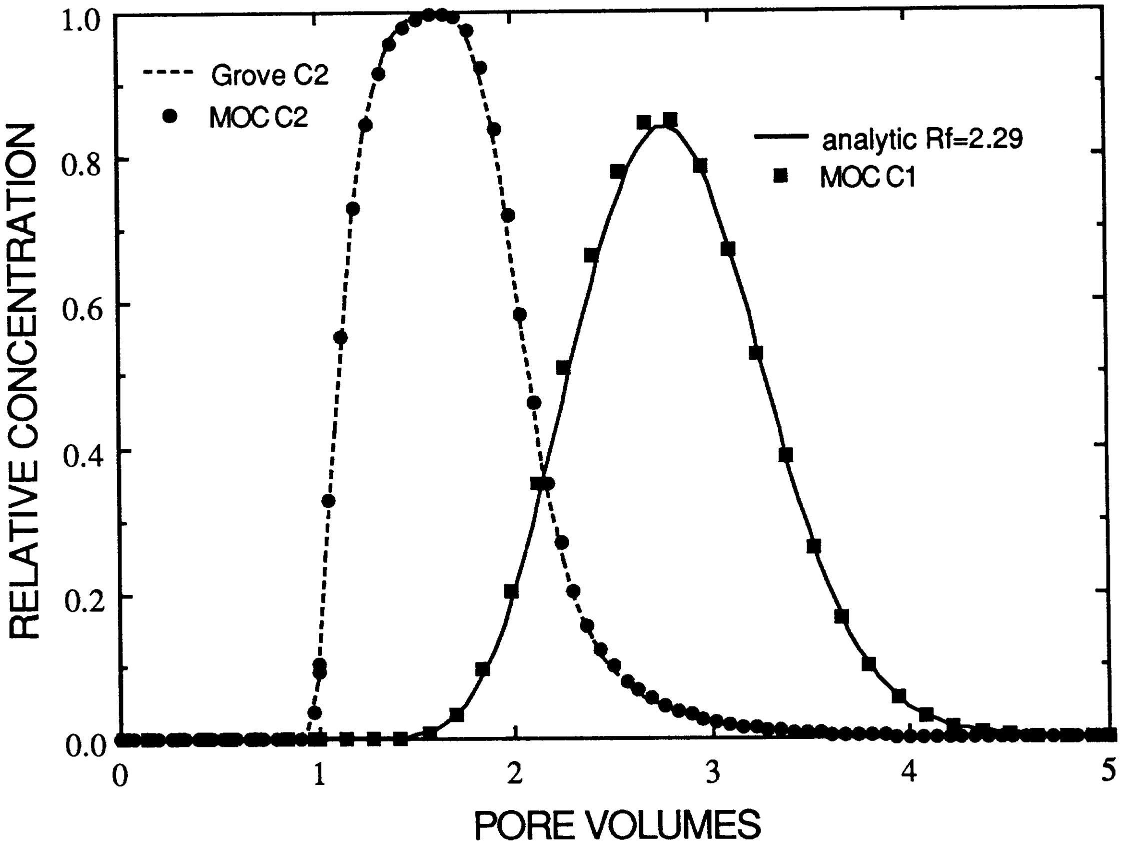

Figure 10. Breakthrough for transport in one-dimensional flow with divalent-monovalent ion exchange ("Grove" is the model of Grove and Stollenwerk (1984), "MOC" is the present work, C1 = input concentration of 0.00005 milligrams per liter, C2 = input concentration of 0.05 milligrams per liter).

Two-dimensional Transport with Sorption and Decay

The model results are also compared to the limiting analytical solution for a two-dimensional steady-state plume that develops in a uniform flow field in which the solute is subject to radioactive decay and linear sorption. In addition, model results are presented for the cases of Freundlich and Langmuir nonlinear sorption with radioactive decay and are compared to results from the two-dimensional finite-element model SUTRA (Voss, 1984). A minor error in the SUTRA program has been corrected so that line 0580 now reads: SL(I)=CHI1*RU (C. I. Voss, U.S. Geological Survey, oral commun., 1988).

For uniform, steady-state flow in the x-direction, the governing equation for transport with linear sorption and decay is (Bear, 1979)

$$R_f \frac{\partial C}{\partial t} = \alpha_L V_x \frac{\partial^2 C}{\partial x^2} + \alpha_T V_x \frac{\partial^2 C}{\partial y^2} - V_x \frac{\partial C}{\partial x} - R_f \lambda C \ , \qquad (38)$$

where α_L is the longitudinal dispersivity, L, and α_T is the transverse dispersivity, L. The analytical solution assumes an infinite domain with injection of chemical mass at $x = y = 0$ at a rate of S. The steady-state analytical solution for the case of constant R_f is (Wilson and Miller, 1978, 1979)

$$C(t \rightarrow \infty) = \frac{S \exp(x/B) K_0(r/B)}{2\pi b \varepsilon V_x (\alpha_L \ \alpha_T)^{1/2}} \ , \qquad (39a)$$

where K_0 is the modified Bessel function of the second kind, and

$$B = 2\alpha_L \ ; \qquad r = \left[\zeta \left(x^2 + \frac{\alpha_L}{\alpha_T} y^2 \right) \right]^{1/2} ; \qquad \zeta = 1 + 2B\lambda R_f / V_x \ . \qquad (39b)$$

The numerical model grid was designed to use symmetry in y to simulate only one-half of the domain. The grid is 67 x 45 cells with $\Delta x = 13.33$ m and $\Delta y = 3.33$ m. The finite-element node spacing is identical. The numerical model boundary conditions are advective flux only, $\partial^2 C/\partial x^2 = 0$ at $x = -220$ m and $x = 673.33$ m, and no transport, $\partial C/\partial y = 0$, at $y = 150$ m and $y = 0$ m. These boundary conditions are sufficiently removed from the source so that concentrations are essentially zero at the boundaries. The steady-state solution with linear sorption given by the model agrees well with the analytical solution and the SUTRA results (fig. 11) for the parameters in table 2. The figure represents contours of equal concentration and the contour label is $\log_{10}(C)$ so that order of magnitude changes can be illustrated. The model presented here (MOC) exhibits excess dispersion upstream of the source which is a result of the decoupled numerical solution scheme in the method-of-characteristics model. Figures 12 and 13 illustrate the affects of Freundlich and Langmuir sorption, respectively, on the steady-state distribution using parameters from table 2. Compared to the linear sorption case (fig. 11), the nonlinear cases have larger areas with high concentrations ($\log_{10}(C)$ greater than 3) but smaller overall dimensions. This steep drop in concentrations is caused by the increased relative sorption and retardation at low concentrations for the nonlinear isotherms. For the two nonlinear cases shown, concentrations agree reasonably well with results from SUTRA, although concentrations differ by up to an order of magnitude at very low concentrations. These differences are probably related to the coarse discretization and the explicit decoupling of the advection and dispersion components in the method-of-characteristics model. Input data and selected program output for the Langmuir sorption example problem with a coarser grid (20x15) are given in appendixes B and C, respectively.

Table 2. -- Parameters for two-dimensional examples

Uniform velocity in x-direction	$V_x = 1$ m/d
Thickness	$b = 10$ m
Porosity	$\varepsilon = 0.1$
Longitudinal dispersivity	$\alpha_L = 20$ m
Transverse dispersivity	$\alpha_T = 2$ m
Dispersion coefficients	$D_{xx} = 20$ m^2/d
	$D_{yy} = 2$ m^2/d
	$D_{xy} = D_{yx} = 0$
Bulk density of porous medium	$\rho_b = 2.16$ g/ml
Source strength	$S = 10^9$ mg/yr
Half-life	$t_{1/2} = 60$ d
Linear sorption equilibrium coefficient	$K_d = 0.1$ ml/g
Freundlich equilibrium coefficient	$K_f = 0.4$
Freundlich slope exponent	$n = 0.7$
Langmuir equilibrium coefficient	$K_\ell = 0.02$ ml/g
Maximum sorption capacity	$Q = 50$ ng/g

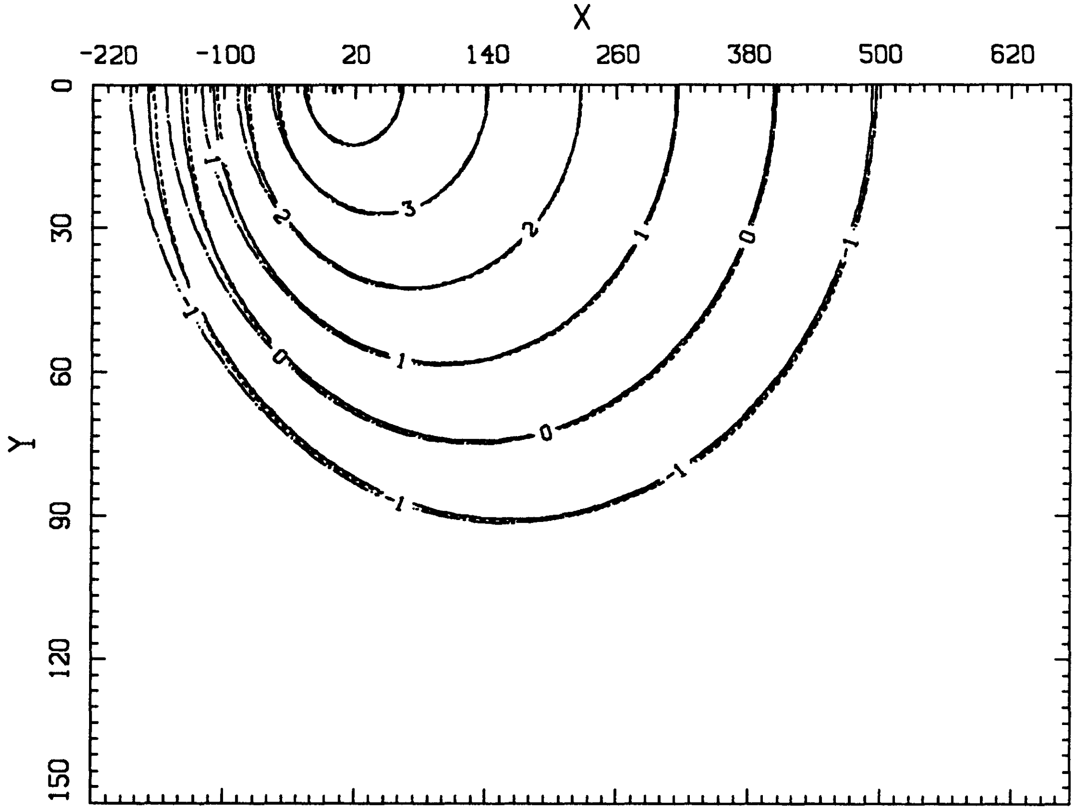

Figure 11. Contours of steady-state plume in a two-dimensional uniform flow-field with linear sorption and decay (Contour labels are $\log_{10}(C)$, analytic solution (solid line), SUTRA solution (dash line), and the present work (dash-dot line)).

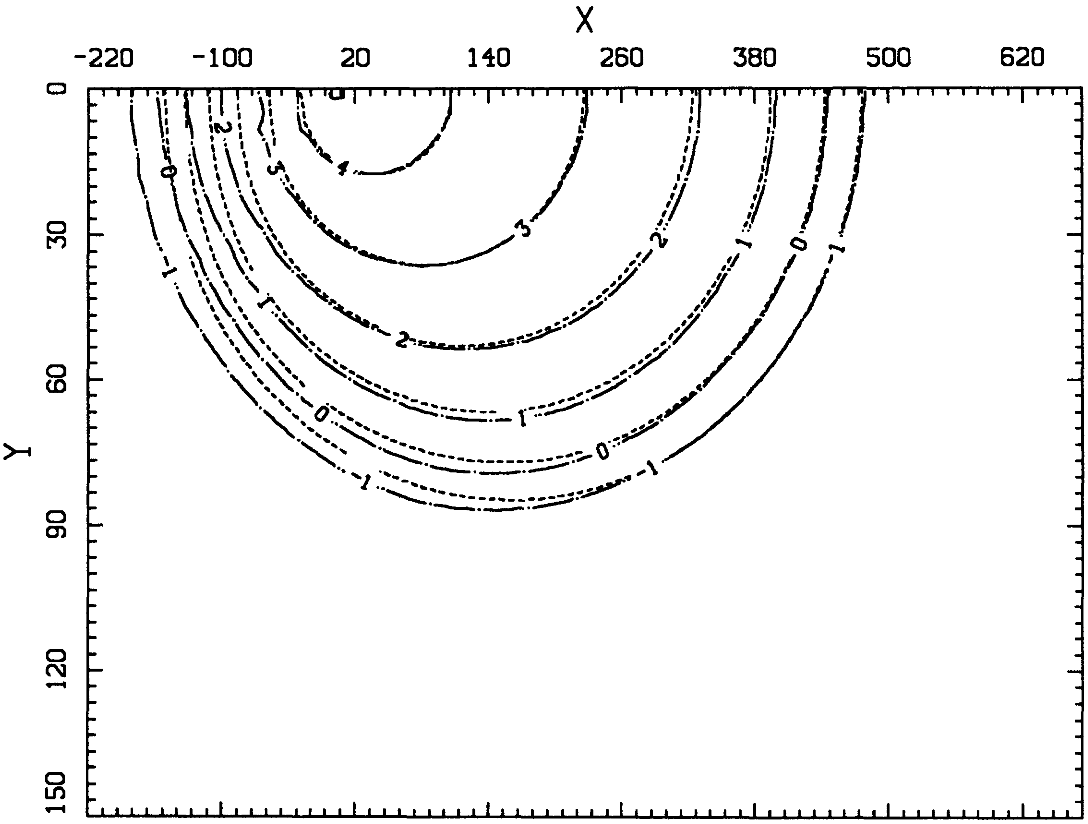

Figure 12. Contours of steady-state plume in a two-dimensional uniform flow-field with Freundlich sorption and decay (Contour labels are $\log_{10}(C)$, analytic solution (solid line), SUTRA solution (dash line), and the present work (dash-dot line)).

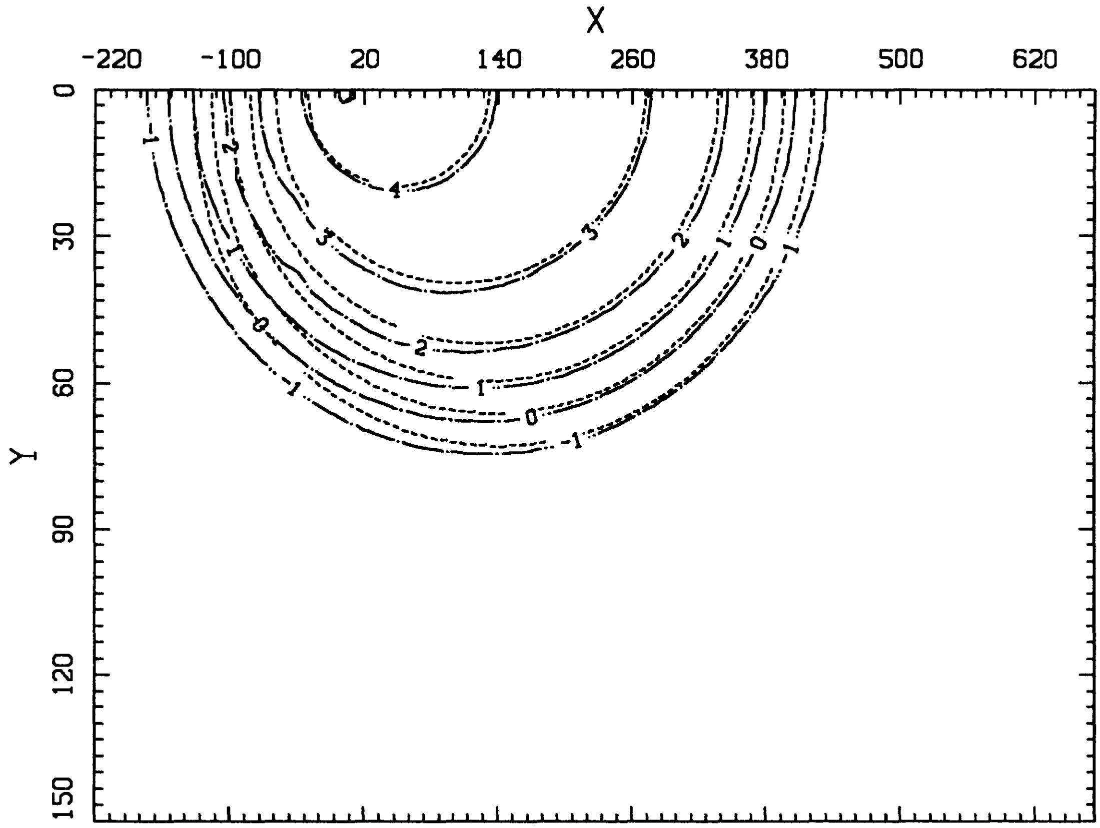

Figure 13. Contours of steady-state plume in a two-dimensional uniform flow-field with Langmuir sorption and decay (Contour labels are $\log_{10}(C)$, analytic solution (solid line), SUTRA solution (dash line), and the present work (dash-dot line)).

SUMMARY AND CONCLUSIONS

A general computer model of solute transport in two-dimensional ground-water systems has been modified to account for the effects of the following processes: irreversible first-order decay; linear equilibrium-controlled sorption; Freundlich equilibrium-controlled sorption; Langmuir equilibrium-controlled sorption; and equilibrium-controlled ion exchange for monovalent-monovalent, divalent-divalent, monovalent-divalent, and divalent-monovalent ion pairs. The assumption of instantaneous and reversible equilibrium allows the mass of solute sorbed or exchanged to be accounted for in the transport equation in terms of the mass dissolved in the water. Thus, only a single transport equation need be solved, greatly reducing computational expense. The assumption of instantaneous and reversible equilibrium may be appropriate for many solute-transport problems, but the validity of this assumption should be evaluated independently for each application.

The modifications to the computer program are relatively minor and straightforward and use algorithms for nonlinear retardation factors developed by Grove and Stollenwerk (1984). The modified version of the model is fully compatible with previous versions; old input files can be used with the new version without changes. This report, the original model documentation (Konikow and Bredehoeft, 1978), and updates (see Preface) provide complete documentation to the model development and application.

The new capabilities of the model were tested by comparison with available analytical solutions (linear sorption and decay) and with other numerical models. Test results indicate the model is performing satisfactorily and as intended.

REFERENCES

Bear, J., 1979, Hydraulics of Groundwater: McGraw-Hill, New York, 567 p.

Charbeneau, R. J., 1981, Groundwater contaminant transport with adsorption and ion exchange chemistry: Method of characteristics for the case without dispersion: Water Resources Research, v. 17, no. 3, p. 705-713.

Freeze, R. A., and Cherry, J. A., 1979, Groundwater: Prentice-Hall, Englewood Cliffs, NJ, 604 p.

Gershon, N. D., and Nir, A., 1969, Effects of boundary conditions of models on tracer distribution in flow through porous mediums: Water Resources Research, v. 5, no. 4, p. 830-839.

Grove, D. B., and Stollenwerk, K. G., 1984, Computer model of one-dimensional equilibrium controlled sorption processes: U.S. Geological Survey Water-Resources Investigations Report 84-4059, 58 p.

Konikow, L. F., and Bredehoeft, J. D., 1978, Computer model of two-dimensional solute transport and dispersion in ground water: U.S. Geological Survey Techniques of Water-Resources Investigations, book 7, chap. C2, 90 p.

Konikow, L. F., and Grove, D. B., 1977, Derivation of equations describing solute transport in ground water: U.S. Geological Survey Water-Resources Investigations Report 77-19, [Revised 1984], 30 p.

Tracy, J. V., 1982, Users guide and documentation for adsorption and decay modifications to the USGS solute transport model: U.S. Nuclear Regulatory Commission Report NUREG/CR-2502, 140 p.

Van Genuchten, M. Th., and Alves, W. J., 1982, Analytical solutions of the one-dimensional convective-dispersive solute transport equation: U.S. Department of Agriculture Technical Bulletin 1661, 151 p.

Voss, C. I., 1984, SUTRA - A finite-element simulation model for saturated-unsaturated, fluid-density-dependent ground-water flow with energy transport or chemically-reactive single-species solute transport: U.S. Geological Survey Water-Resources Investigations Report 84-4369, 409 p.

Wilson, J. L., and Miller, P. J., 1978, Two-dimensional plume in uniform ground-water flow: American Society of Civil Engineers, Journal of Hydraulics Division, v. 104, no. HY4, p. 503-514.

Wilson, J. L., and Miller, P. J., 1979, Two-dimensional plume in uniform ground-water flow--Closure: American Society of Civil Engineers, Journal of Hydraulics Division, v. 105, no. HY12, p. 1567-1570.

APPENDIX A

COMPUTER-PROGRAM MODIFICATIONS

These modifications allow simulation of solutes affected by the following chemical interactions: nonlinear Freundlich or Langmuir equilibrium-controlled sorption; and monovalent and divalent equilibrium-controlled ion exchange. Prior to implementing these changes, the program should be updated through November 21, 1988.

These modifications can be implemented as follows (note line numbers in columns 73-80):

FILE A: Previous version updated through November 21, 1988
FILE B: New modified version

```
           1         2         3         4         5         6         7         8
  12345678901234567890123456789012345678901234567890123456789012345678901234567890
           |         |         |         |         |         |         |         |

INSERT
B-C     *    REV. MARCH 1989 BY D.J. GOODE FOR NONLINEAR EQUILIBRIUM    *   A  68C
B-C     *     SORPTION AND ION-EXCHANGE FOR MONO AND DIVALENT IONS      *   A  68D


A-      COMMON /CHMR/ RF,DK,RHOB,THALF,DECAY,ADSORB,SORBI,DMASS1,CSTM2      A 238R
CHANGED TO
B-      COMMON /CHMR/ RF,DK,RHOB,THALF,DECAY,ADSORB,SORBI,DMASS1,CSTM2,     A 238A
B-     1              EKF,XNF,XNFM1,FCTRF,EKL,CEC,EKLCEC,FCTRL,CINMAX,      A 238B
B-     2        RF2MIN,RF2MAX,CZERO,IREACT,EK,EKCEC,FCTRE,CTOT,C3,C4,C5,C6  A 238C
B-      COMMON /CHMR2/ CRETRD(020,020),CRDCOF(020,020),CELDCY(020,020)      A 238D


INSERT
B-      CHARACTER*26 REACTN(9)                                              B  67R


A-      COMMON /CHMR/ RF,DK,RHOB,THALF,DECAY,ADSORB,SORBI,DMASS1,CSTM2      B 182R
CHANGED TO
B-      COMMON /CHMR/ RF,DK,RHOB,THALF,DECAY,ADSORB,SORBI,DMASS1,CSTM2,     B 181R
B-     1              EKF,XNF,XNFM1,FCTRF,EKL,CEC,EKLCEC,FCTRL,CINMAX,      B 183R
B-     2        RF2MIN,RF2MAX,CZERO,IREACT,EK,EKCEC,FCTRE,CTOT,C3,C4,C5,C6  B 184R


INSERT
B-      DATA REACTN/                  'NONE                      ',         B 213R
B-     1 'LINEAR SORPTION           ','FREUNDLICH SORPTION       ',         B 214R
B-     2 'LANGMUIR SORPTION         ','MONOVALENT ION EXCHANGE   ',         B 215R
B-     3 'DIVALENT ION EXCHANGE     ','MONO-DIVALENT ION EXCHANGE',         B 216R
B-     4 'DI-MONOVALENT ION EXCHANGE','DECAY ONLY                '/         B 217R


INSERT
B-      CINMAX=0.0                                                          B 298R
```

```
           1         2         3         4         5         6         7         8
  12345678901234567890123456789012345678901234567890123456789012345678901234567890
           |         |         |         |         |         |         |         |
INSERT
B-      EKF=0.0                                                             B 301R
B-      EKL=0.0                                                             B 302R
B-      EK=0.0                                                              B 303R
B-      XNF=1.0                                                             B 304R
B-      CEC=0.0                                                             B 305R
B-      CTOT=0.0                                                            B 306R
B-      RF2MIN=1.0                                                          B 307R
B-      RF2MAX=1.0                                                          B 308R


A-     1PND,NCODES,NPNTMV,NPNTVL,NPNTD,NPDELC,NPNCHV,NREACT                 B 431R
CHANGED TO
B-     1PND,NCODES,NPNTMV,NPNTVL,NPNTD,NPDELC,NPNCHV,IREACT                 B 431A


A-      IF (NREACT.EQ.1) READ (5,*) DK,RHOB,THALF                           B 455R
CHANGED TO
B-      IF (IREACT.EQ.1) READ (5,*) DK,RHOB,THALF                           B 456R
B-      IF (IREACT.LT.-1.OR.IREACT.GT.7) IREACT=0                           B 457R
B-      IF (IREACT.EQ.-1) READ (5,*) THALF                                  B 458R
B-      IF (IREACT.EQ.2) READ (5,*) RHOB,EKF,XNF,THALF                      B 459R
B-      IF (IREACT.EQ.3) READ (5,*) RHOB,EKL,CEC,THALF                      B 461R
B-      IF (IREACT.GE.4) READ (5,*) RHOB,EK,CEC,CTOT,THALF                  B 462R
B-      XNFM1=XNF-1.                                                        B 463R
B-      FCTRF=RHOB*EKF*XNF/POROS                                            B 464R
B-      EKLCEC=EKL*CEC                                                      B 465R
B-      FCTRL=RHOB*EKLCEC/POROS                                             B 466R
B-      EKCEC=EK*CEC                                                        B 467R
B-      IF (CTOT.GT.0.0) FCTRE=RHOB*EKCEC/(POROS*CTOT)                      B 468A
B-      C3=RHOB/POROS                                                       B 468B
B-      C4=EKCEC                                                            B 468C
B-      C5=C4*CEC                                                           B 468D
B-      C6=CTOT*CTOT                                                        B 468E
B-C      CZERO IS THE MINIMUM CONC. LEVEL FOR NONLINEAR RETARDATION         B 468F
B-      CZERO=0.9E-15                                                       B 468G
B-      CALL RETRD2(1.E-15,RF2MAX,RDCOEF)                                   B 468H
B-      CZERO=1.E-15                                                        B 469R

A-     1PDELC                                                               B 630
A-      WRITE (6,895) DK,RHOB,RF,THALF,DECAY                                B 635R
CHANGED TO
B-     1PDELC,IREACT                                                        B 631R
B-      IF (IREACT.EQ.-1) THEN                                              B 632A
B-       WRITE (6,891) REACTN(9)                                            B 632B
B-       IREACT=0                                                           B 632C
B-      ELSE                                                                B 632D
B-       WRITE (6,891) REACTN(IREACT+1)                                     B 632E
B-      END IF                                                              B 632F
B-      IF (IREACT.GE.1) THEN                                               B 633R
B-       WRITE (6,892) RHOB                                                 B 634R
B-       IF (IREACT.EQ.1) THEN                                              B 636R
B-        WRITE (6,893) DK,RF                                               B 637R
B-       ELSE                                                               B 638R
B-        IF (IREACT.EQ.2) WRITE (6,894) EKF,XNF                            B 639R
B-        IF (IREACT.EQ.3) WRITE (6,895) EKL,CEC                            B 641R
B-        IF (IREACT.GE.4) WRITE (6,896) EK,CEC,CTOT                        B 642R
B-        IF (BETA.EQ.0.0) WRITE (6,897)                                    B 643R
B-       END IF                                                             B 644R
B-      END IF                                                              B 645R
B-      IF (DECAY.NE.0.0) WRITE (6,898) THALF,DECAY                         B 646R
```

```
           1         2         3         4         5         6         7         8
  12345678901234567890123456789012345678901234567890123456789012345678901234567890
           |         |         |         |         |         |         |         |

A-      IF (NREC.GT.0) THEN                                                 B 703
CHANGED TO
B-C        AND RESET MINIMUM RETARDATION                                    B 703A
B-      IF (NREC.GT.0.OR.(IREACT.GE.2.AND.IREACT.LE.7)) THEN                B 703B
B-       CINMAX=0.0                                                         B 703C


A-       IF (REC(IX,IY).EQ.0.0) GO TO 12                                    B 705A
CHANGED TO
B-      JX=IX-MX+1                                                         SB 704C
B-      JY=IY-MY+1                                                         SB 704D
B-       IF (REC(IX,IY).NE.0.0) THEN                                        B 704E


DELETE
A-        JX=IX-MX+1                                                       SB 706A
A-        JY=IY-MY+1                                                       SB 706B


INSERT
B-       END IF                                                             B 707C
B-       IF (JX.GT.0.AND.JX.LE.NMX.AND.JY.GT.0.AND.JY.LE.NMY) THEN         SB 707D
B-        IF (CONC(JX,JY).GT.CINMAX) CINMAX=CONC(JX,JY)                    SB 707E
B-        IF ((VPRM(IX,IY).NE.0.0.OR.RECH(JX,JY).LT.0.0)                   SB 707F
B-     1         .AND.CNRECH(JX,JY).GT.CINMAX)  CINMAX=CNRECH(JX,JY)       SB 707G
B-       END IF                                                             B 707H


INSERT
B-       CALL RETRD2(CINMAX,RF2MIN,RDCOEF)                                  B 708A
B-       IF (IREACT.EQ.2.AND.XNFM1.GT.0.0) RF2MIN=RF2MAX                    B 708B


A-      IF (INT.GT.1.AND.ICHK.LE.0) RETURN                                  B1345
CHANGED TO
B-      IF (INT.GT.1.AND.ICHK.LE.0) THEN                                    B1346A
B-       IF (IREACT.GE.2.AND.IREACT.LE.7) WRITE (6,899) RF2MIN              B1346B
B-       RETURN                                                             B1346C
B-      END IF                                                              B1346D


INSERT
B-      IF (FCTR.LT.0.0.AND.CNREC.GT.CINMAX) CINMAX=CNREC                   B1384R


INSERT
B-      CALL RETRD2(CINMAX,RF2MIN,RDCOEF)                                   B1404R
B-      IF (IREACT.EQ.2.AND.XNFM1.GT.0.0) RF2MIN=RF2MAX                     B1405R


A-  120 IF (INT.GT.1) RETURN                                                B1420
CHANGED TO
B-  120 IF (INT.GT.1) THEN                                                  B1421R
B-       IF (IREACT.GE.2.AND.IREACT.LE.7) WRITE (6,899) RF2MIN              B1422R
B-       RETURN                                                             B1423R
B-      END IF                                                              B1424R


INSERT
B-      IF (FCTR2.GT.CINMAX) CINMAX=FCTR2                                   B2553R
```

```
           1         2         3         4         5         6         7         8
  12345678901234567890123456789012345678901234567890123456789012345678901234567890
           |         |         |         |         |         |         |         |


INSERT
B-      IF (IREACT.GE.2)                                                    B3095A
B-     1    SORBI=SORBI+RHOB/POROS*AREA*THCK(JX,JY)*SORB2(CONINT(IX,IY))   SB3095B
B-      IF (CONINT(IX,IY).GT.CINMAX) CINMAX=CONINT(IX,IY)                   B3095C


INSERT
B-      CALL RETRD2(CINMAX,RF2MIN,RDCOEF)                                   B3112R
B-      IF (IREACT.EQ.2.AND.XNFM1.GT.0.0) RF2MIN=RF2MAX                     B3113R
B-      IF (IREACT.GE.2.AND.IREACT.LE.7) WRITE (6,899) RF2MIN               B3114R


A-     4 13X,'NPDELC (PRINT OPT.-CONC. CHANGE) =  ',I4)                     B4119
A-  895 FORMAT (1H0,23X,14HREACTION TERMS//13X,37HDK      (DISTRIBUTION CO  B4121R
A-     1EFFICIENT) = ,E12.5/13X,37HRHOB    (BULK DENSITY OF SOLIDS)   = ,E  B4122R
A-     212.5/13X,37HRF       (RETARDATION FACTOR)        = ,E12.5/13X,37HTHA  B4123R
A-     3LF   (HALF LIFE OF DECAY,IN SEC)= ,E12.5/13X,37HDECAY   (DECAY CON  B4124R
A-     4STANT=LN 2/THALF)= ,E12.5)                                          B4125R
CHANGED TO
B-     4 13X,'NPDELC (PRINT OPT.-CONC. CHANGE) =  ',I4/                     B4118R
B-     5 13X,'IREACT (REACTION SPECIFIER)      = ',I5)                      B4126R
B-  891 FORMAT (//13X,'REACTION - ',A26/)                                   B4127R
B-  892 FORMAT (13X,'RHOB    (BULK DENSITY)                  = ',1PE12.5)   B4128A
B-  893 FORMAT (13X,'DK      (DISTRIBUTION COEFFICIENT)      = ',1PE12.5/   B4128B
B-     1        13X,'RF      (RETARDATION FACTOR)            = ',1PE12.5)   B4128C
B-  894 FORMAT (13X,'EKF     (FREUNDLICH SORPTION CONSTANT)= ',1PE12.5/     B4128D
B-     1        13X,'XNF     (FREUNDLICH SORPTION SLOPE)     = ',1PE12.5)   B4128E
B-  895 FORMAT (13X,'EKL     (LANGMUIR SORPTION CONSTANT)    = ',1PE12.5/   B4128F
B-     1        13X,'CEC     (CATION EXCHANGE CAPACITY)      = ',1PE12.5)   B4128G
B-  896 FORMAT (13X,'EK      (ION EXCHANGE CONSTANT)         = ',1PE12.5/   B4128H
B-     1        13X,'CEC     (CATION EXCHANGE CAPACITY)      = ',1PE12.5/   B4128I
B-     2        13X,'CTOT    (TOTAL SOLUTE CONCENTRATION)    = ',1PE12.5)   B4128J
B-  897 FORMAT (/' *** WARNING ***  BETA.EQ.0.0 AND SORPTION-EXCHANGE IS',  B4129A
B-     1                                         ' NONLINEAR')              B4129B
B-  898 FORMAT (/13X,'THALF   (HALF LIFE OF DECAY,IN SEC)    = ',1PE12.5/   B4129C
B-     1         13X,'DECAY   (DECAY CONSTANT=LN 2/THALF)    = ',1PE12.5)   B4129D
B-  899 FORMAT (1H0,' MINIMUM NONLINEAR RETARDATION FACTOR FOR THIS',       B4129E
B-     1            ' PUMPING PERIOD'//10X,' RF2MIN = ',1PE12.4)            B4129F


A-      COMMON /CHMR/ RF,DK,RHOB,THALF,DECAY,ADSORB,SORBI,DMASS1,CSTM2      E 205R
CHANGED TO
B-      COMMON /CHMR/ RF,DK,RHOB,THALF,DECAY,ADSORB,SORBI,DMASS1,CSTM2,     E 206R
B-     1              EKF,XNF,XNFM1,FCTRF,EKL,CEC,EKLCEC,FCTRL,CINMAX,      E 207R
B-     2        RF2MIN,RF2MAX,CZERO,IREACT,EK,EKCEC,FCTRE,CTOT,C3,C4,C5,C6  E 208R


A-      TDIV=(THCK(IX,IY)*RF)/DABS(DIV)                                     E 712R
CHANGED TO
B-      TDIV=THCK(IX,IY)/DABS(DIV)                                          E 712


A-   20 CONTINUE                                                            E 730
CHANGED TO
B-   20 CONTINUE                                                            E 728
B-      TMV=TMV*RF*RF2MIN                                                   E 729R
```

```
           1         2         3         4         5         6         7         8
  12345678901234567890123456789012345678901234567890123456789012345678901234567890
           |         |         |         |         |         |         |         |

A-      IF (RF.LE.1.0) GO TO 115                                            E1071R
A-      VMXBD=VMXBD/RF                                                      E1075R
A-      VMYBD=VMYBD/RF                                                      E1076R
CHANGED TO
B-      IF (IREACT.LE.0) GO TO 115                                          E1072R
B-      VMXBD=VMXBD/(RF*RF2MIN)                                             E1077R
B-      VMYBD=VMYBD/(RF*RF2MIN)                                             E1078R


A-      TIMDC=0.5*RF/TIMDIS                                                 E1851R
CHANGED TO
B-      TIMDC=0.5*RF*RF2MIN/TIMDIS                                          E1852R


A-      COMMON /CHMR/ RF,DK,RHOB,THALF,DECAY,ADSORB,SORBI,DMASS1,CSTM2      F 172R
CHANGED TO
B-      COMMON /CHMR/ RF,DK,RHOB,THALF,DECAY,ADSORB,SORBI,DMASS1,CSTM2,     F 173R
B-     1              EKF,XNF,XNFM1,FCTRF,EKL,CEC,EKLCEC,FCTRL,CINMAX,      F 174A
B-     2        RF2MIN,RF2MAX,CZERO,IREACT,EK,EKCEC,FCTRE,CTOT,C3,C4,C5,C6  F 174B
B-      COMMON /CHMR2/ CRETRD(020,020),CRDCOF(020,020),CELDCY(020,020)      F 175R


INSERT
B-      DO 8 IY=1,NMY                                                       F 269A
B-      JY=IY+MY-1                                                         SF 269B
B-      DO 8 IX=1,NMX                                                       F 269C
B-      JX=IX+MX-1                                                         SF 269D
B-      CRETRD(IX,IY)=1.0                                                   F 269E
B-      CRDCOF(IX,IY)=1.0                                                   F 269F
B-      CELDCY(IX,IY)=1.0                                                   F 269G
B-      IF (IREACT.LE.1.OR.THCK(JX,JY).EQ.0.0) GO TO 8                     SF 269H
B-      CALL RETRD2(CONC(IX,IY),CRETRD(IX,IY),CRDCOF(IX,IY))                F 269I
B-      IF (DECAY.NE.0.0)                                                   F 269J
B-     1    CELDCY(IX,IY)=EXP(-DCYFCT*CRDCOF(IX,IY)/CRETRD(IX,IY))          F 269K
B-    8 CONTINUE                                                            F 269L


INSERT
B-      IF (IREACT.GE.2) THEN                                               F2052R
B-       RF2INV=1.0/CRETRD(JX,JY)                                          SF2053R
B-       DISTX=DISTX*RF2INV                                                 F2054R
B-       DISTY=DISTY*RF2INV                                                 F2055R
B-      ENDIF                                                               F2056R


INSERT
B-      IF (DECAY.NE.0.0) THEN                                              F2415A
B-       IF (IREACT.LE.1) THEN                                              F2415B


INSERT
B-       ELSE                                                               F2417R
B-        PART(3,IN)=PART(3,IN)*CELDCY(JX,JY)                              SF2418A
B-       END IF                                                             F2418B
B-      END IF                                                              F2419R
```

```
         1         2         3         4         5         6         7         8
12345678901234567890123456789012345678901234567890123456789012345678901234567890
         |         |         |         |         |         |         |         |

A-   398 SUMC(JX,JY)=SUMC(JX,JY)+CONC(JX,JY)*DCYT2                          SF2868R
CHANGED TO
B-   398 IF (IREACT.LE.1) THEN                                               F2864R
B-        SUMC(JX,JY)=SUMC(JX,JY)+CONC(JX,JY)*DCYT2                         SF2865R
B-       ELSE                                                                F2866R
B-        SUMC(JX,JY)=SUMC(JX,JY)+CONC(JX,JY)*SQRT(CELDCY(JX,JY))           SF2867R
B-       END IF                                                              F2869R


A-       PART(3,IP)=CONC(JX,JY)*DCYT                                        SF3478
CHANGED TO
B-       IF (IREACT.LE.1) THEN                                               F3478A
B-        PART(3,IP)=CONC(JX,JY)*DCYT                                       SF3478B
B-       ELSE                                                                F3478C
B-        PART(3,IP)=CONC(JX,JY)*CELDCY(JX,JY)                              SF3478D
B-       END IF                                                              F3478E


A-       COMMON /CHMR/ RF,DK,RHOB,THALF,DECAY,ADSORB,SORBI,DMASS1,CSTM2      G 195R
CHANGED TO
B-       COMMON /CHMR/ RF,DK,RHOB,THALF,DECAY,ADSORB,SORBI,DMASS1,CSTM2,     G 196R
B-      1              EKF,XNF,XNFM1,FCTRF,EKL,CEC,EKLCEC,FCTRL,CINMAX,      G 197R
B-      2        RF2MIN,RF2MAX,CZERO,IREACT,EK,EKCEC,FCTRE,CTOT,C3,C4,C5,C6  G 198R
B-       COMMON /CHMR2/ CRETRD(020,020),CRDCOF(020,020),CELDCY(020,020)      G 199R


A-       EQFCT=RFFCT/THCK(JX,JY)                                            SG 383R
CHANGED TO
B-       CALL RETRD2(CAVG(IX,IY),RF2,RDCOEF)                                 G 384R
B-       EQFCT=RFFCT/(THCK(JX,JY)*RF2)                                      SG 385R


A-       C1=EXP((ALOG(CNOLD(IX,IY))+ALOG(CONC(IX,IY)))*0.5)                  G 488R
CHANGED TO
B-C      NEXT CALC IS EQUIVALENT TO C1=EXP((ALOG(CNOLD)+ALOG(CONC))*0.5)     G 488A
B-       C1=SQRT(CNOLD(IX,IY)*CONC(IX,IY))                                   G 488B


INSERT
B-       ADSRB2=0.0                                                          G1412R


A-       DELDCY=CNOLD(IX,IY)-CNOLD(IX,IY)*DCYT                               G1444A
CHANGED TO
B-       IF (DECAY.NE.0.0) THEN                                              G1445A
B-        DELDCY=CNOLD(IX,IY)*(1.0-DCYT)                                     G1445B
B-        IF (IREACT.GE.2) DELDCY=DELDCY+SORB2(CNOLD(IX,IY))*(1.0-DCYT)*C3   G1445C


INSERT
B-       END IF                                                              G1447R


INSERT
B-       IF (IREACT.GE.2) ADSRB2=ADSRB2+THCK(JX,JY)*SORB2(C1)               SG1475R
```

```
           1         2         3         4         5         6         7         8
  12345678901234567890123456789012345678901234567890123456789012345678901234567890
           |         |         |         |         |         |         |         |

INSERT
B-      IF (IREACT.GE.2) THEN                                               G1686R
B-       CALL RETRD2(C1,CRETRD(IX,IY),CRDCOF(IX,IY))                        G1687A
B-       IF (DECAY.NE.0.0)                                                  G1687B
B-     1     CELDCY(IX,IY)=EXP(-DCYFCT*CRDCOF(IX,IY)/CRETRD(IX,IY))         G1687C
B-      END IF                                                              G1688R


A-      ADSORB=ADSORB*DK*RHOB/POROS*AREA                                    G1718R
CHANGED TO
B-      ADSORB=(ADSORB*DK+ADSRB2)*RHOB/POROS*AREA                           G1719R


A-      COMMON /CHMR/ RF,DK,RHOB,THALF,DECAY,ADSORB,SORBI,DMASS1,CSTM2      I 155R
CHANGED TO
B-      COMMON /CHMR/ RF,DK,RHOB,THALF,DECAY,ADSORB,SORBI,DMASS1,CSTM2,     I 156R
B-     1              EKF,XNF,XNFM1,FCTRF,EKL,CEC,EKLCEC,FCTRL,CINMAX,      I 157R
B-     2        RF2MIN,RF2MAX,CZERO,IREACT,EK,EKCEC,FCTRE,CTOT,C3,C4,C5,C6  I 158R


ADD AT END
B-C     ***  RETRD2  *****************************************************   K  10
B-C                                                                         K  20
B-      SUBROUTINE RETRD2(CONC,RF2,RDCOEF)                                  K  30
B-C                                                                         K  40
B-C     ******************************************************************   K  50
B-      DOUBLE PRECISION AA,BB,CC,QUADX                                     K  60
B-      COMMON /CHMR/ RF,DK,RHOB,THALF,DECAY,ADSORB,SORBI,DMASS1,CSTM2,     K  70
B-     1              EKF,XNF,XNFM1,FCTRF,EKL,CEC,EKLCEC,FCTRL,CINMAX,      K  80
B-     2        RF2MIN,RF2MAX,CZERO,IREACT,EK,EKCEC,FCTRE,CTOT,C3,C4,C5,C6  K  90
B-C     ******************************************************************   K 100
B-C     ---COMPUTE NONLINEAR RETARDATION FACTOR (RF2) AND CORRECTION TERM   K 110
B-C          FOR DECAY OF SORBED SOLUTE (RDCOEF)---                         K 120
B-C                                                                         K 130
B-      RF2=1.0                                                             K 140
B-      RDCOEF=1.0                                                          K 150
B-      IF (IREACT.LE.1) RETURN                                             K 160
B-      C=CONC                                                              K 170
B-      IF (C.LE.CZERO) THEN                                                K 180
B-       RF2=RF2MAX                                                         K 190
B-       RDCOEF=RF2MAX                                                      K 200
B-       RETURN                                                             K 210
B-      END IF                                                              K 220
B-C                                                                         K 230
B-C     ---FREUNDLICH ISOTHERM---                                           K 240
B-      IF (IREACT.EQ.2) THEN                                               K 250
B-       TERM=FCTRF*C**XNFM1                                                K 260
B-       RF2=1.+TERM                                                        K 270
B-       RDCOEF=1.+TERM/XNF                                                 K 280
B-C                                                                         K 290
B-C     ---LANGMUIR ISOTHERM---                                             K 300
B-      ELSE IF (IREACT.EQ.3) THEN                                          K 310
B-       DINV=1./(1.+EKL*C)                                                 K 320
B-       TERM=FCTRL*DINV                                                    K 330
B-       RF2=1.+TERM*DINV                                                   K 340
B-       RDCOEF=1.+TERM                                                     K 350
B-C                                                                         K 360
B-C     ---MONOVALENT ION EXCHANGE---                                       K 370
B-      ELSE IF (IREACT.EQ.4) THEN                                          K 380
B-       RF2=1.+FCTRE/((C/CTOT*(EK-1.)+1.)**2)                              K 390
```

```
             1         2         3         4         5         6         7         8
    12345678901234567890123456789012345678901234567890123456789012345678901234567890
             |         |         |         |         |         |         |         |

B-         RDCOEF=1.+FCTRE*CTOT/((CTOT-C)+EK*C)
B-C
B-C       ---DIVALENT ION EXCHANGE---
B-        ELSE IF (IREACT.EQ.5) THEN
B-         CTOT2=CTOT*0.5
B-         RF2=1.+FCTRE/((C/CTOT2*(EK-1.)+1.)**2)
B-         RDCOEF=1.+FCTRE*CTOT2/((CTOT2-C)+EK*C)
B-C
B-C       ---MONOVALENT-DIVALENT ION EXCHANGE---
B-        ELSE IF (IREACT.EQ.6) THEN
B-         C2=C*C
B-         AA=CTOT-C
B-         BB=C2*EK
B-         CC=-EKCEC*C2
B-         CBAR=QUADX(AA,BB,CC,1.D0)
B-         RDCOEF=1.+C3*CBAR/C
B-         DCBAR=(CBAR*CBAR-CBAR*2.*C*EK+2.*C*EKCEC)/
B-       1       ((CTOT-C)*2.*CBAR+C2*EK)
B-         RF2=1.+C3*DCBAR
B-C
B-C       ---DIVALENT-MONOVALENT ION EXCHANGE---
B-        ELSE
B-         C2=C*C
B-         AA=4.D0*EK*C
B-         BB=-4.D0*C4*C-C6+4.D0*C*CTOT-C2*4.D0
B-         CC=C5*C
B-         CBAR=QUADX(AA,BB,CC,-1.D0)
B-         RDCOEF=1.+C3*CBAR/C
B-         A=(-4.*CBAR*CBAR*EK-CBAR*(-4.*C4+4.*CTOT-8.*C)-C5)
B-         B=(4.*EK*C*(2.*CBAR-CEC)-C6+4.*C*CTOT-4.*C2)
B-         IF (B.EQ.0.0) THEN
B-          RF2=1.+C3*1.E-10
B-         ELSE
B-          RF2=1.+C3*A/B
B-         END IF
B-        END IF
B-        RETURN
B-        END
B-C       ***  SORB2  *****************************************************
B-C
B-        FUNCTION SORB2(CONC)
B-C
B-C       *****************************************************************
B-        DOUBLE PRECISION AA,BB,CC,QUADX
B-        COMMON /CHMR/ RF,DK,RHOB,THALF,DECAY,ADSORB,SORBI,DMASS1,CSTM2,
B-       1              EKF,XNF,XNFM1,FCTRF,EKL,CEC,EKLCEC,FCTRL,CINMAX,
B-       2        RF2MIN,RF2MAX,CZERO,IREACT,EK,EKCEC,FCTRE,CTOT,C3,C4,C5,C6
B-C       *****************************************************************
B-C       ---SORB2 IS SORBED CONCENTRATION CORRESPONDING TO CONC IN SOLUTION
B-C
B-        SORB2=0.0
B-        IF (IREACT.LE.1) RETURN
B-        C=CONC
B-        IF (C.LE.CZERO) RETURN
B-C
B-C       ---FREUNDLICH ISOTHERM---
B-        IF (IREACT.EQ.2) THEN
B-         SORB2=EKF*C**XNF
B-C
B-C       ---LANGMUIR ISOTHERM---
```

```
             1         2         3         4         5         6         7         8
    12345678901234567890123456789012345678901234567890123456789012345678901234567890
             |         |         |         |         |         |         |         |
B-        ELSE IF (IREACT.EQ.3) THEN                                          K1000
B-         SORB2=EKLCEC*C/(1.+EKL*C)                                          K1010
B-C                                                                           K1020
B-C       ---MONOVALENT ION EXCHANGE---                                       K1030
B-        ELSE IF (IREACT.EQ.4) THEN                                          K1040
B-         SORB2=EKCEC*C/(C*(EK-1.)+CTOT)                                     K1050
B-C                                                                           K1060
B-C       ---DIVALENT ION EXCHANGE---                                         K1070
B-        ELSE IF (IREACT.EQ.5) THEN                                          K1080
B-         SORB2=EKCEC*C/(2.*C*(EK-1.)+CTOT)                                  K1090
B-C                                                                           K1100
B-C       ---MONOVALENT-DIVALENT ION EXCHANGE---                              K1110
B-        ELSE IF (IREACT.EQ.6) THEN                                          K1120
B-         AA=CTOT-C                                                          K1130
B-         C2=C*C                                                             K1140
B-         BB=C2*EK                                                           K1150
B-         CC=-EKCEC*C2                                                       K1160
B-         SORB2=QUADX(AA,BB,CC,1.D0)                                         K1170
B-C                                                                           K1180
B-C       ---DIVALENT-MONOVALENT ION EXCHANGE---                              K1190
B-        ELSE                                                                K1200
B-         AA=4.D0*EK*C                                                       K1210
B-         C2=C*C                                                             K1220
B-         BB=-4.D0*C4*C-C6+4.D0*C*CTOT-C2*4.D0                               K1230
B-         CC=C5*C                                                            K1240
B-         SORB2=QUADX(AA,BB,CC,-1.D0)                                        K1250
B-        END IF                                                              K1260
B-        RETURN                                                              K1270
B-        END                                                                 K1280
B-C       ***  QUADX  ******************************************************  K1290
B-C                                                                           K1300
B-        DOUBLE PRECISION FUNCTION QUADX(A,B,C,D)                            K1310
B-C                                                                           K1320
B-C       ******************************************************************  K1330
B-        DOUBLE PRECISION A,B,C,D,T                                          K1340
B-C       ---SOLVE QUADRATIC EQUATION---                                      K1350
B-        T=B*B-4.D0*A*C                                                      K1360
B-        IF (T.LT.0.0) THEN                                                  K1370
B-         QUADX=-B/(2.D0*A)                                                  K1380
B-        ELSE                                                                K1390
B-         QUADX=(-B+D*DSQRT(T))/(2.D0*A)                                     K1400
B-        END IF                                                              K1410
B-        RETURN                                                              K1420
B-        END                                                                 K1430
```

APPENDIX B

INPUT DATA FOR A SAMPLE PROBLEM

```
         1         2         3         4         5         6         7         8
12345678901234567890123456789012345678901234567890123456789012345678901234567890
         |         |         |         |         |         |         |         |

TWO-D PLUME IN STEADY FLOW, LANGMUIR SORPTION WITH DECAY   NOV 88
   1   1 -24 176400   1   7   0 200   0  16   3  40   0   0   0   0   3
  2  2   21  16
  4.0 1E-8 0.10 20.0  0.0  0.0  0.0 40.0 10.0  0.1 0.25  1.0
  2.16  0.02  50.0  5.184E6
01.15741E-3
0  10.
0  0.0
1  1.0
0000000000000000000
0000
0100002000000000000
0310
0100000000000000000
0010
0100000000000000000
0010
0100000000000000000
0010
0100000000000000000
0010
0100000000000000000
0010
0100000000000000000
0010
0100000000000000000
0010
0100000000000000000
0010
0100000000000000000
0010
0100000000000000000
0010
0100000000000000000
0010
0100000000000000000
0010
0100000000000000000
0010
0000000000000000000
0000
 1   1.0       0.0       0.0    0
 2   0.0       3.171E7  -1.25E-91
 3   0.0           0.0   1.25E-91
1  1.0
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0
 0.0 9.4 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 1.0 0.0
 0.0 9.4 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 1.0 0.0
```

```
         1         2         3         4         5         6         7         8
12345678901234567890123456789012345678901234567890123456789012345678901234567890
         |         |         |         |         |         |         |         |

 0.0 9.4 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 1.0 0.0
 0.0 9.4 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 1.0 0.0
 0.0 9.4 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 1.0 0.0
 0.0 9.4 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 1.0 0.0
 0.0 9.4 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 1.0 0.0
 0.0 9.4 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 1.0 0.0
 0.0 9.4 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 1.0 0.0
 0.0 9.4 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 1.0 0.0
 0.0 9.4 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 1.0 0.0
 0.0 9.4 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 1.0 0.0
 0.0 9.4 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 1.0 0.0
 0.0 9.4 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 1.0 0.0
 0.0 9.4 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 1.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0
0  0.0
```

APPENDIX C

SELECTED OUTPUT FROM A SAMPLE PROBLEM

APPENDIX C

Selected Output from a Sample Problem

```
U.S.G.S. METHOD-OF-CHARACTERISTICS MODEL FOR SOLUTE TRANSPORT IN GROUND WATER

TWO-D PLUME IN STEADY FLOW, LANGMUIR SORPTION WITH DECAY   NOV 88

                 I N P U T    D A T A

                   GRID DESCRIPTORS

         NX    (NUMBER OF COLUMNS)  =    24
         NY    (NUMBER OF ROWS)     =    17
         XDEL  (X-DISTANCE IN FEET) =    40.0
         YDEL  (Y-DISTANCE IN FEET) =    10.0

              SECONDARY SUBGRID FOR TRANSPORT

            NMX   (NUMBER OF COLUMNS)  =    20
            NMY   (NUMBER OF ROWS)     =    15

            CROSS-REF. TO PRIMARY GRID      IX  IY
                                            --- ---
              FIRST NODE (UPPER LEFT) AT:    2   2
              LAST NODE (LOWER RIGHT) AT:   21  16

                   TIME  PARAMETERS

         NTIM   (MAX. NO. OF TIME STEPS)       =      1
         NPMP   (NO. OF PUMPING PERIODS)       =      1
         PINT   (PUMPING PERIOD IN YEARS)      =      4.000
         TIMX   (TIME INCREMENT MULTIPLIER)    =      0.00
         TINIT  (INITIAL TIME STEP IN SEC.)    =      0.

          HYDROLOGIC AND CHEMICAL PARAMETERS

         S       (STORAGE COEFFICIENT)       =      0.000000
         POROS   (EFFECTIVE POROSITY)        =      0.100
         BETA    (LONGITUDINAL DISPERSIVITY) =     20.0
         DLTRAT  (RATIO OF TRANSVERSE TO
                 LONGITUDINAL DISPERSIVITY)  =      0.10
         ANFCTR  (RATIO OF T-YY TO T-XX)     =      1.000000

                 EXECUTION PARAMETERS

         NITP   (NO. OF ITERATION PARAMETERS) =    7
         TOL    (CONVERGENCE CRITERIA - ADIP) =  0.10E-07
         ITMAX  (MAX.NO.OF ITERATIONS - ADIP) =  200
         CELDIS (MAX.CELL DISTANCE PER MOVE
                    OF PARTICLES - M.O.C.)    =    0.100
         NPMAX  (MAX. NO. OF PARTICLES)       = 6400
         NPTPND (NO. PARTICLES PER NODE)      =    16
```

```
                PROGRAM OPTIONS

          NPNT    (TIME STEP INTERVAL FOR
                   COMPLETE PRINTOUT)        =     1
          NPNTMV  (MOVE INTERVAL FOR CHEM.
                   CONCENTRATION PRINTOUT)   =    40
          NPNTVL  (TIME STEP INTERVAL FOR
                   VELOCITY PRINTOUT; 0=NEVER;
                   -1=FIRST TIME STEP;
                   -2=LAST TIME STEP)        =     0
          NPNTD   (PRINT OPTION-DISP.COEF.
                   0=NO; 1=FIRST TIME STEP;
                   2=ALL TIME STEPS)         =     0
          NUMOBS  (NO. OF OBSERVATION WELLS
                   FOR HYDROGRAPH PRINTOUT) =     0
          NREC    (NO. OF PUMPING WELLS)     =     0
          NCODES  (FOR NODE IDENT.)          =     3
          NPNCHV  (TIME STEP INTERVAL FOR
                   VELOCITY PRINTOUT ON
                   FILE UNIT 7; 0=NEVER;
                   -1=FIRST TIME STEP;
                   -2=LAST TIME STEP)        =     0
          NPDELC  (PRINT OPT.-CONC. CHANGE) =     0
          IREACT  (REACTION SPECIFIER)       =     3


          REACTION - LANGMUIR SORPTION

          RHOB     (BULK DENSITY)                  =  2.16000E+00
          EKL      (LANGMUIR SORPTION CONSTANT)   =  2.00000E-02
          CEC      (CATION EXCHANGE CAPACITY)     =  5.00000E+01

          THALF    (HALF LIFE OF DECAY,IN SEC)    =  5.18400E+06
          DECAY    (DECAY CONSTANT=LN 2/THALF)    =  1.33709E-07


            STEADY-STATE FLOW

 TIME INTERVALS (IN SEC) FOR SOLUTE-TRANSPORT SIMULATION
0.12623E+09

       AREA OF ONE CELL =     400.0

       X-Y SPACING:
            40.000
            10.000
```

```
TRANSMISSIVITY MAP (FT*FT/SEC)

    0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01
    0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01
    0.00E-01  0.00E-01  0.00E-01  0.00E-01
    0.00E-01  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03
    1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03
    1.16E-03  1.16E-03  1.16E-03  0.00E-01
     .         .         .         .         .         .         .         .         .         .
     .         .         .         .         .         .         .         .         .         .
     .         .         .         .         .         .         .         .         .         .
    0.00E-01  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03
    1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03  1.16E-03
    1.16E-03  1.16E-03  1.16E-03  0.00E-01
    0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01
    0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01
    0.00E-01  0.00E-01  0.00E-01  0.00E-01

AQUIFER THICKNESS (FT)

     0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
     0.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0  0.0
      .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .
      .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .
      .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .
     0.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0  0.0
     0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0

DIFFUSE RECHARGE AND DISCHARGE (FT/SEC)

    0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01
    0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01
    0.00E-01  0.00E-01  0.00E-01  0.00E-01
     .         .         .         .         .         .         .         .         .         .
     .         .         .         .         .         .         .         .         .         .
     .         .         .         .         .         .         .         .         .         .
    0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01
    0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01
    0.00E-01  0.00E-01  0.00E-01  0.00E-01

PERMEABILTY MAP (FT/SEC)

    0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01
    0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01
    0.00E-01  0.00E-01  0.00E-01  0.00E-01
    0.00E-01  1.16E-04  1.16E-04  1.16E-04  1.16E-04  1.16E-04  1.16E-04  1.16E-04  1.16E-04  1.16E-04
    1.16E-04  1.16E-04  1.16E-04  1.16E-04  1.16E-04  1.16E-04  1.16E-04  1.16E-04  1.16E-04  1.16E-04
    1.16E-04  1.16E-04  1.16E-04  0.00E-01
     .         .         .         .         .         .         .         .         .         .
     .         .         .         .         .         .         .         .         .         .
```

```
      .          .          .          .          .          .          .          .          .          .
      .          .          .          .          .          .          .          .          .          .
  0.00E-01   1.16E-04   1.16E-04   1.16E-04   1.16E-04   1.16E-04   1.16E-04   1.16E-04   1.16E-04   1.16E-04
  1.16E-04   1.16E-04   1.16E-04   1.16E-04   1.16E-04   1.16E-04   1.16E-04   1.16E-04   1.16E-04   1.16E-04
  1.16E-04   1.16E-04   1.16E-04   0.00E-01
  0.00E-01   0.00E-01   0.00E-01   0.00E-01   0.00E-01   0.00E-01   0.00E-01   0.00E-01   0.00E-01   0.00E-01
  0.00E-01   0.00E-01   0.00E-01   0.00E-01   0.00E-01   0.00E-01   0.00E-01   0.00E-01   0.00E-01   0.00E-01
  0.00E-01   0.00E-01   0.00E-01   0.00E-01

 FLOW MODEL (PRIMARY GRID):

          NO. OF FINITE-DIFFERENCE CELLS IN AQUIFER =  330

          AREA OF AQUIFER IN MODEL   =  0.13200E+06   SQ. FT.

 TRANSPORT SUBGRID:

          NO. OF FINITE-DIFFERENCE CELLS IN AQUIFER =  300

          AREA OF AQUIFER IN MODEL   =  0.12000E+06   SQ. FT.

          NZCRIT   (MAX. NO. OF CELLS THAT CAN BE VOID OF
                    PARTICLES;  IF EXCEEDED, PARTICLES ARE REGENERATED)   =    6

NODE IDENTIFICATION MAP

   0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
   0  1  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  3  1  0
   0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0
   0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0
   .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .
   .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .
   .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .
   0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0
   0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0

    NO. OF NODE IDENT. CODES SPECIFIED =  3

          THE FOLLOWING ASSIGNMENTS HAVE BEEN MADE:
    CODE NO.      LEAKANCE      SOURCE CONC.      RECHARGE

        1         0.100E+01          0.00

        2         0.000E+00     *********
                                                  -0.125E-08

        3         0.000E+00          0.00
                                                   0.125E-08
```

```
VERTICAL PERMEABILITY/THICKNESS (FT/(FT*SEC))

   0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01
   0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01
   0.00E-01  0.00E-01  0.00E-01  0.00E-01
   0.00E-01  1.00E+00  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01
   0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01
   0.00E-01  0.00E-01  1.00E+00  0.00E-01
    .         .         .         .         .         .         .         .         .         .
    .         .         .         .         .         .         .         .         .         .
    .         .         .         .         .         .         .         .         .         .
   0.00E-01  1.00E+00  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01
   0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01
   0.00E-01  0.00E-01  1.00E+00  0.00E-01
   0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01
   0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01  0.00E-01
   0.00E-01  0.00E-01  0.00E-01  0.00E-01

WATER TABLE

    0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
    0.   0.   0.   0.
    0.   9.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
    0.   0.   1.   0.
     .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .
     .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .
     .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .    .
    0.   9.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
    0.   0.   1.   0.
    0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
    0.   0.   0.   0.

HEAD DISTRIBUTION - ROW
 NUMBER OF TIME STEPS =      0
        TIME(SECONDS) =  0.00000
        TIME(DAYS)    =  0.00000E+00
        TIME(YEARS)   =  0.00000E+00

   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000
   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000
   0.0000000   0.0000000   0.0000000   0.0000000
   0.0000000   9.4000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000
   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000
   0.0000000   0.0000000   1.0000000   0.0000000
    .           .           .           .           .           .           .           .           .           .
    .           .           .           .           .           .           .           .           .           .
    .           .           .           .           .           .           .           .           .           .
   0.0000000   9.4000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000
   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000
   0.0000000   0.0000000   1.0000000   0.0000000
   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000
   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000
   0.0000000   0.0000000   0.0000000   0.0000000
```

```
ITERATION PARAMETERS
           0.100444E-02
           0.317397E-02
           0.100296E-01
           0.316929E-01
           0.100148
           0.316461
            1.00000

 MINIMUM NONLINEAR RETARDATION FACTOR FOR THIS PUMPING PERIOD

           RF2MIN =    1.0000E+00


CONCENTRATION

 NUMBER OF TIME STEPS =      0
        TIME(SECONDS) =  0.00000
   CHEM.TIME(SECONDS) =  0.00000E+00
   CHEM.TIME(DAYS)    =  0.00000E+00
        TIME(YEARS)   =  0.00000E+00
   CHEM.TIME(YEARS)   =  0.00000E+00
  NO. MOVES COMPLETED =      0

    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0


   N =     1
   NUMBER OF ITERATIONS =    42

HEAD DISTRIBUTION - ROW
 NUMBER OF TIME STEPS =      1
        TIME(SECONDS) =  0.12623E+09
        TIME(DAYS)    =  0.14610E+04
        TIME(YEARS)   =  0.40000E+01
```

```
   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000
   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000
   0.0000000   0.0000000   0.0000000   0.0000000
   0.0000000   9.3999997   9.0000855   8.6001745   8.2002727   7.8003995   7.4006546   7.0004483   6.6003703   6.2003210
   5.8002814   5.4002456   5.0002114   4.6001780   4.2001448   3.8001116   3.4000780   3.0000432   2.6000053   2.1999595
   1.7998888   1.3996995   1.0000003   0.0000000
   0.0000000   9.3999997   9.0000853   8.6001739   8.2002709   7.8003915   7.4005755   7.0004403   6.6003685   6.2003204
   5.8002811   5.4002455   5.0002114   4.6001780   4.2001449   3.8001117   3.4000781   3.0000434   2.6000058   2.1999611
   1.7998962   1.3997768   1.0000003   0.0000000
   0.0000000   9.3999997   9.0000850   8.6001728   8.2002677   7.8003795   7.4005163   7.0004283   6.6003652   6.2003192
   5.8002807   5.4002453   5.0002113   4.6001780   4.2001449   3.8001117   3.4000782   3.0000438   2.6000068   2.1999639
   1.7999071   1.3998328   1.0000003   0.0000000
     .           .           .           .           .           .           .           .           .           .
     .           .           .           .           .           .           .           .           .           .
     .           .           .           .           .           .           .           .           .           .
   0.0000000   9.3999997   9.0000782   8.6001544   8.2002250   7.8002840   7.4003222   7.0003326   6.6003223   6.2003002
   5.8002722   5.4002416   5.0002098   4.6001775   4.2001451   3.8001129   3.4000812   3.0000505   2.6000221   2.1999984
   1.7999837   1.3999840   1.0000003   0.0000000
   0.0000000   9.3999997   9.0000779   8.6001537   8.2002235   7.8002814   7.4003189   7.0003300   6.6003207   6.2002994
   5.8002719   5.4002414   5.0002097   4.6001775   4.2001451   3.8001130   3.4000813   3.0000508   2.6000227   2.1999995
   1.7999855   1.3999857   1.0000003   0.0000000
   0.0000000   9.3999997   9.0000777   8.6001533   8.2002228   7.8002802   7.4003173   7.0003288   6.6003200   6.2002990
   5.8002717   5.4002413   5.0002097   4.6001775   4.2001451   3.8001130   3.4000814   3.0000510   2.6000230   2.2000001
   1.7999864   1.3999866   1.0000003   0.0000000
   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000
   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000
   0.0000000   0.0000000   0.0000000   0.0000000


HEAD DISTRIBUTION - ROW
 NUMBER OF TIME STEPS =      1
        TIME(SECONDS) =  0.12623E+09
        TIME(DAYS)    =  0.14610E+04
        TIME(YEARS)   =  0.40000E+01

   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0
   0   9   9   9   8   8   7   7   7   6   6   5   5   5   4   4   3   3   3   2   2   1   1   0
   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .
   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .
   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .
   0   9   9   9   8   8   7   7   7   6   6   5   5   5   4   4   3   3   3   2   2   1   1   0
   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0


DRAWDOWN
       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
       0    0   -9   -9   -8   -8   -7   -7   -7   -6   -6   -5   -5   -5   -4   -4   -3   -3   -3   -2   -2   -1    0    0
       .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .
       .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .
       .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .   .
       0    0   -9   -9   -8   -8   -7   -7   -7   -6   -6   -5   -5   -5   -4   -4   -3   -3   -3   -2   -2   -1    0    0
       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
```

```
 CUMULATIVE MASS BALANCE -- (IN FT**3)

   RECHARGE AND INJECTION      = -0.63115E+02
   PUMPAGE AND E-T WITHDRAWAL =  0.63115E+02
   CUMULATIVE  NET  PUMPAGE   =  0.00000E+00
   WATER RELEASE FROM STORAGE =  0.00000E+00
   LEAKAGE INTO AQUIFER       =  0.21911E+06
   LEAKAGE OUT OF AQUIFER     = -0.21911E+06
   CUMULATIVE  NET  LEAKAGE   =  0.50299E+00

      MASS BALANCE RESIDUAL  =  0.50299
       ERROR  (AS PERCENT)    =  0.22950E-03


 RATE MASS BALANCE -- (IN C.F.S.)


   LEAKAGE INTO AQUIFER       =  0.17358E-02
   LEAKAGE OUT OF AQUIFER     = -0.17358E-02
   NET LEAKAGE    (QNET)      =  0.39847E-08
   RECHARGE AND INJECTION     = -0.50000E-06
   PUMPAGE AND E-T WITHDRAWAL =  0.50000E-06
   NET WITHDRAWAL   (TPUM)    =  0.00000E+00

          STABILITY CRITERIA --- M.O.C.


    MAXIMUM FLUID VELOCITIES:  X-VEL =  1.16E-05     Y-VEL =  9.16E-09

    MAXIMUM EFFECTIVE SOLUTE VELOCITIES:  X-VEL =  1.16E-05     Y-VEL =  9.16E-09

TMV (MAX. INJ.) =  0.34567E+07
 TIMV (CELDIS)   =  0.34542E+06

TIMV =  3.45E+05     NTIMV =   365     NMOV =   366

  TIM (N)  =  0.12623E+09
  TIMEVELO =  0.34489E+06
  TIMEDISP =  0.13287E+07

TIMV =  3.45E+05     NTIMD =    95     NMOV =   366

          THE LIMITING STABILITY CRITERION IS CELDIS
    MAX. X-VEL. IS CONSTRAINT AND OCCURS BETWEEN NODES ( 7, 2) AND ( 8, 2)

          NO. OF PARTICLE MOVES REQUIRED TO COMPLETE THIS TIME STEP  =  366


 NP        =         4800          IMOV      =            1
  TIM(N)   =  0.12623E+09           TIMV     =  0.34489E+06          SUMTCH =  0.34489E+06
 NP        =         4800          IMOV      =            2
  TIM(N)   =  0.12623E+09           TIMV     =  0.34489E+06          SUMTCH =  0.68978E+06
```

```
NP          =         4800          IMOV      =          3
 TIM(N)     =  0.12623E+09           TIMV     =  0.34489E+06          SUMTCH =  0.10347E+07
NP          =         4800          IMOV      =          4
 TIM(N)     =  0.12623E+09           TIMV     =  0.34489E+06          SUMTCH =  0.13796E+07
NP          =         4800          IMOV      =          5
 TIM(N)     =  0.12623E+09           TIMV     =  0.34489E+06          SUMTCH =  0.17245E+07
      .       .       .       .       .       .       .       .       .       .       .
      .       .       .       .       .       .       .       .       .       .       .
      .       .       .       .       .       .       .       .       .       .       .
NP          =         4800          IMOV      =         17
 TIM(N)     =  0.12623E+09           TIMV     =  0.34489E+06          SUMTCH =  0.58632E+07
NP          =         4800          IMOV      =         18
   NUMBER OF CELLS WITH ZERO PARTICLES  =      1     IMOV   =    18

 TIM(N)     =  0.12623E+09           TIMV     =  0.34489E+06          SUMTCH =  0.62080E+07
NP          =         4800          IMOV      =         19
   NUMBER OF CELLS WITH ZERO PARTICLES  =      1     IMOV   =    19

 TIM(N)     =  0.12623E+09           TIMV     =  0.34489E+06          SUMTCH =  0.65529E+07
NP          =         4800          IMOV      =         20
 TIM(N)     =  0.12623E+09           TIMV     =  0.34489E+06          SUMTCH =  0.68978E+07
NP          =         4800          IMOV      =         21
 TIM(N)     =  0.12623E+09           TIMV     =  0.34489E+06          SUMTCH =  0.72427E+07
      .       .       .       .       .       .       .       .       .       .       .
      .       .       .       .       .       .       .       .       .       .       .
      .       .       .       .       .       .       .       .       .       .       .
NP          =         4800          IMOV      =         40
   NUMBER OF CELLS WITH ZERO PARTICLES  =      4     IMOV   =    40

 TIM(N)     =  0.12623E+09           TIMV     =  0.34489E+06          SUMTCH =  0.13796E+08


CONCENTRATION

 NUMBER OF TIME STEPS =      1
       DELTA T        =  0.12623E+09
       TIME(SECONDS)  =  0.12623E+09
  CHEM.TIME(SECONDS)  =  0.13796E+08
  CHEM.TIME(DAYS)     =  0.15967E+03
       TIME(YEARS)    =  0.40000E+01
  CHEM.TIME(YEARS)    =  0.43716E+00
 NO. MOVES COMPLETED  =    40

   0    1   74 1904 813966052428811941411649 4723 1476  318    2    0    0    0    0    0    0    0
   0    0   14  850 3893171871983711729 6088 3023  921  105    1    0    0    0    0    0    0    0
   0    0    1   73 1327 2045 5521 5331 3023 1371  377   21    0    0    0    0    0    0    0    0
   0    0    0    2  117  971 1309 1481  942  307   34    0    0    0    0    0    0    0    0    0
   0    0    0    0    2   36   82   83   27    4    0    0    0    0    0    0    0    0    0    0
   0    0    0    0    0    1    1    1    0    0    0    0    0    0    0    0    0    0    0    0
   0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
   0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
   0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
   0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
```

```
   0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
   0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
   0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
   0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
   0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0

CHEMICAL MASS BALANCE

       MASS IN BOUNDARIES     =  0.00000E+00
       MASS OUT BOUNDARIES    = -0.41201E-13
       MASS PUMPED IN         =  0.21873E+09
       MASS PUMPED OUT        =  0.00000E+00
       MASS LOST BY DECAY     = -0.11313E+09
       MASS ADSORBED ON SOLIDS=  0.14629E+08
       INITIAL MASS ADSORBED  =  0.00000E+00
       INFLOW MINUS OUTFLOW   =  0.21873E+09
       INITIAL MASS DISSOLVED =  0.00000E+00
       PRESENT MASS DISSOLVED =  0.97907E+08
       CHANGE MASS DISSOLVED  =  0.97907E+08
       CHANGE TOTL.MASS STORED=  0.11254E+09
     COMPARE RESIDUAL WITH NET FLUX AND MASS ACCUMULATION:
       MASS BALANCE RESIDUAL  = -0.69393E+07
       ERROR  (AS PERCENT)    = -0.31725E+01

 NP      =         4800          IMOV     =          41
    NUMBER OF CELLS WITH ZERO PARTICLES  =     4    IMOV   =    41

  TIM(N)   =  0.12623E+09          TIMV     =  0.34489E+06         SUMTCH =  0.14141E+08
 NP      =         4800          IMOV     =          42
    NUMBER OF CELLS WITH ZERO PARTICLES  =     3    IMOV   =    42

  TIM(N)   =  0.12623E+09          TIMV     =  0.34489E+06         SUMTCH =  0.14485E+08
      .       .       .       .       .       .       .       .       .       .       .
      .       .       .       .       .       .       .       .       .       .       .
      .       .       .       .       .       .       .       .       .       .       .
 NP      =         4800          IMOV     =          58
    NUMBER OF CELLS WITH ZERO PARTICLES  =     4    IMOV   =    58

  TIM(N)   =  0.12623E+09          TIMV     =  0.34489E+06         SUMTCH =  0.20004E+08
 NP      =         4800          IMOV     =          59
    NUMBER OF CELLS WITH ZERO PARTICLES  =     7    IMOV   =    59

    ***   NZCRIT EXCEEDED  ---  CALL GENPT   ***

 NPCELL

    16 16  4  8  4  0  4  8  8  8 12 20 92 24 16 16 16 16 16 16
    16 16 12  4  0  4  8  8  0 16  8 28 84 20 16 16 16 16 16 16
    16 16 16  0 12  4  4  0 12  4 20 76 28 16 16 16 16 16 16 16
    16 16 16 16  0  8  8  0 12 16 56 28 16 16 16 16 16 16 16 16
    16 16 16 16 16  8  8 12 24 24 20 16 16 16 16 16 16 16 16 16
    16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16
    16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16
```

```
       16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16
       16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16
       16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16
       16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16
       16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16
       16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16
       16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16
       16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16 16
  TIM(N)   =  0.12623E+09         TIMV     =  0.34489E+06         SUMTCH =  0.20349E+08
 NP        =         4800        IMOV     =            60
  TIM(N)   =  0.12623E+09         TIMV     =  0.34489E+06         SUMTCH =  0.20693E+08
 NP        =         4800        IMOV     =            61
  TIM(N)   =  0.12623E+09         TIMV     =  0.34489E+06         SUMTCH =  0.21038E+08
      .       .       .       .       .       .       .       .       .       .       .
      .       .       .       .       .       .       .       .       .       .       .
      .       .       .       .       .       .       .       .       .       .       .
 NP        =         4800        IMOV     =            80
    NUMBER OF CELLS WITH ZERO PARTICLES  =     3     IMOV   =    80

  TIM(N)   =  0.12623E+09         TIMV     =  0.34489E+06         SUMTCH =  0.27591E+08


 CONCENTRATION

  NUMBER OF TIME STEPS =      1
         DELTA T       =  0.12623E+09
         TIME(SECONDS) =  0.12623E+09
    CHEM.TIME(SECONDS) =  0.27591E+08
    CHEM.TIME(DAYS)    =  0.31934E+03
         TIME(YEARS)   =  0.40000E+01
    CHEM.TIME(YEARS)   =  0.87431E+00
   NO. MOVES COMPLETED =     80

    0   11  336 1371 733356928385042192613194 6708 3571 1745  691  137    9    0    0    0    0    0
    0    4   86  752 3465140291859814306 9191 5214 2856 1420  491   86    3    0    0    0    0    0
    0    1   21  164 1486 3708 6888 6951 5081 3186 1793  845  250   35    2    0    0    0    0    0
    0    0    3   52  349 1375 2047 2674 2223 1493  830  338   81    4    0    0    0    0    0    0
    0    0    0    5   48  274  554  743  661  437  207   48    5    0    0    0    0    0    0    0
    0    0    0    0    3   14   36   61   51   26    9    1    0    0    0    0    0    0    0    0
    0    0    0    0    0    1    1    2    1    1    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
```

```
CHEMICAL MASS BALANCE

       MASS IN BOUNDARIES     =  0.00000E+00
       MASS OUT BOUNDARIES    = -0.41926E-07
       MASS PUMPED IN         =  0.43746E+09
       MASS PUMPED OUT        =  0.00000E+00
       MASS LOST BY DECAY     = -0.35056E+09
       MASS ADSORBED ON SOLIDS=  0.21959E+08
       INITIAL MASS ADSORBED  =  0.00000E+00
      .INFLOW MINUS OUTFLOW   =  0.43746E+09
       INITIAL MASS DISSOLVED =  0.00000E+00
       PRESENT MASS DISSOLVED =  0.10721E+09
       CHANGE MASS DISSOLVED  =  0.10721E+09
       CHANGE TOTL.MASS STORED=  0.12917E+09
     COMPARE RESIDUAL WITH NET FLUX AND MASS ACCUMULATION:
       MASS BALANCE RESIDUAL  = -0.42273E+08
       ERROR  (AS PERCENT)    = -0.96633E+01

 NP      =        4800        IMOV     =          81
    NUMBER OF CELLS WITH ZERO PARTICLES  =     1     IMOV   =    81

  TIM(N)   =  0.12623E+09          TIMV     =  0.34489E+06          SUMTCH =  0.27936E+08
      .       .       .       .       .       .       .       .       .       .       .
      .       .       .       .       .       .       .       .       .       .       .
      .       .       .       .       .       .       .       .       .       .       .
 NP      =        4800        IMOV     =         360
    NUMBER OF CELLS WITH ZERO PARTICLES  =     1     IMOV   =   360

  TIM(N)   =  0.12623E+09          TIMV     =  0.34489E+06          SUMTCH =  0.12416E+09


CONCENTRATION

 NUMBER OF TIME STEPS =      1
        DELTA T       =  0.12623E+09
        TIME(SECONDS) =  0.12623E+09
   CHEM.TIME(SECONDS) =  0.12416E+09
   CHEM.TIME(DAYS)    =  0.14370E+04
        TIME(YEARS)   =  0.40000E+01
   CHEM.TIME(YEARS)   =  0.39343E+01
  NO. MOVES COMPLETED =   360

    1   16  317 1303 903955708429991987112419 6915 3844 2083 1014  387   74   10    1    0    0    0
    0    5  112  744 4057148891996413272 8500 5208 3004 1631  798  271   50    6    0    0    0    0
    0    1   28   87 1362 4433 7255 6467 4661 3098 1870 1036  463  125   20    1    0    0    0    0
    0    0    4   77  378 1254 2306 2489 2038 1437  888  462  167   46    7    0    0    0    0    0
    0    0    0    6   59  197  538  713  649  462  253  112   34    8    1    0    0    0    0    0
    0    0    0    0    4   22   62   85   78   56   31   13    3    1    0    0    0    0    0    0
    0    0    0    0    0    1    4    5    6    4    2    1    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
```

```
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0

 CHEMICAL MASS BALANCE

        MASS IN BOUNDARIES      =  0.00000E+00
        MASS OUT BOUNDARIES     = -0.74317E+01
        MASS PUMPED IN          =  0.19686E+10
        MASS PUMPED OUT         =  0.00000E+00
        MASS LOST BY DECAY      = -0.20872E+10
        MASS ADSORBED ON SOLIDS=  0.24272E+08
        INITIAL MASS ADSORBED   =  0.00000E+00
        INFLOW MINUS OUTFLOW    =  0.19686E+10
        INITIAL MASS DISSOLVED =  0.00000E+00
        PRESENT MASS DISSOLVED =  0.10975E+09
        CHANGE MASS DISSOLVED   =  0.10975E+09
        CHANGE TOTL.MASS STORED=  0.13403E+09
      COMPARE RESIDUAL WITH NET FLUX AND MASS ACCUMULATION:
        MASS BALANCE RESIDUAL   = -0.25262E+09
        ERROR  (AS PERCENT)     = -0.12832E+02

 NP        =          4800         IMOV      =          361
    NUMBER OF CELLS WITH ZERO PARTICLES  =     1     IMOV   =    361

  TIM(N)    =  0.12623E+09          TIMV      =  0.34489E+06          SUMTCH =  0.12450E+09
 NP        =          4800         IMOV      =          362
    NUMBER OF CELLS WITH ZERO PARTICLES  =     1     IMOV   =    362

  TIM(N)    =  0.12623E+09          TIMV      =  0.34489E+06          SUMTCH =  0.12485E+09
 NP        =          4800         IMOV      =          363
    NUMBER OF CELLS WITH ZERO PARTICLES  =     1     IMOV   =    363

  TIM(N)    =  0.12623E+09          TIMV      =  0.34489E+06          SUMTCH =  0.12519E+09
 NP        =          4800         IMOV      =          364
    NUMBER OF CELLS WITH ZERO PARTICLES  =     1     IMOV   =    364

  TIM(N)    =  0.12623E+09          TIMV      =  0.34489E+06          SUMTCH =  0.12554E+09
 NP        =          4800         IMOV      =          365
  TIM(N)    =  0.12623E+09          TIMV      =  0.34489E+06          SUMTCH =  0.12588E+09
 NP        =          4800         IMOV      =          366
  TIM(N)    =  0.12623E+09          TIMV      =  0.34489E+06          SUMTCH =  0.12623E+09
```

```
CONCENTRATION

 NUMBER OF TIME STEPS =      1
       DELTA T        =  0.12623E+09
       TIME(SECONDS)  =  0.12623E+09
  CHEM.TIME(SECONDS)  =  0.12623E+09
  CHEM.TIME(DAYS)     =  0.14610E+04
       TIME(YEARS)    =  0.40000E+01
  CHEM.TIME(YEARS)    =  0.39999E+01
 NO. MOVES COMPLETED  =    366

    1   15   47 1454 681244367485452271913822 6981 4132 2187  958  330   79   10    1    0    0    0
    0    5   89  602 3967131091870414914 9323 5612 3240 1666  731  261   61    5    0    0    0    0
    0    1   23  169 1344 3650 6303 6829 5097 3355 2040 1023  442  136   23    2    0    0    0    0
    0    0    4   52  239  890 2122 2486 2195 1492  873  465  177   41    6    0    0    0    0    0
    0    0    0    6   52  248  549  706  663  473  253  111   35    7    1    0    0    0    0    0
    0    0    0    0    4   21   56   89   84   59   29   12    3    1    0    0    0    0    0    0
    0    0    0    0    0    1    4    6    6    4    2    1    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0

 CHEMICAL MASS BALANCE

       MASS IN BOUNDARIES      =  0.00000E+00
       MASS OUT BOUNDARIES     = -0.76534E+01
       MASS PUMPED IN          =  0.20014E+10
       MASS PUMPED OUT         =  0.00000E+00
       MASS LOST BY DECAY      = -0.21242E+10
       MASS ADSORBED ON SOLIDS=  0.24055E+08
       INITIAL MASS ADSORBED   =  0.00000E+00
       INFLOW MINUS OUTFLOW    =  0.20014E+10
       INITIAL MASS DISSOLVED =  0.00000E+00
       PRESENT MASS DISSOLVED =  0.10788E+09
       CHANGE MASS DISSOLVED   =  0.10788E+09
       CHANGE TOTL.MASS STORED=  0.13194E+09
     COMPARE RESIDUAL WITH NET FLUX AND MASS ACCUMULATION:
       MASS BALANCE RESIDUAL   = -0.25474E+09
       ERROR  (AS PERCENT)     = -0.12728E+02
```

(p. 65 follows)

APPENDIX D

ADDITIONAL INPUT FORMATS FOR DECAY, SORPTION, AND ION-EXCHANGE REACTIONS

IREACT is added to an existing card (line):

Card	Columns	Format	Variable	Definition
2	69-72	I4	IREACT	Reaction type specifier

Card 3.1 is inserted after card 3 if IREACT is not 0 or blank:

IREACT	Reaction	Parameters on card 3.1 in free format
-1	decay only	THALF
0	no reaction	do not insert card 3.1
1	linear sorption	DK, RHOB, THALF
2	Freundlich sorption	RHOB, EKF, XNF, THALF
3	Langmuir sorption	RHOB, EKL, CEC, THALF
4	monovalent exchange	RHOB, EK, CEC, CTOT, THALF
5	divanlent exchange	RHOB, EK, CEC, CTOT, THALF
6	mono-divalent exchange	RHOB, EK, CEC, CTOT, THALF
7	di-monovalent exchange	RHOB, EK, CEC, CTOT, THALF

Parameter	Definition
THALF	$t_{1/2}$ - Decay half-life, in seconds, T (if no decay, specify THALF=0.0)
RHOB	ρ_b - aquifer bulk density, mass of solid per unit volume of aquifer, ML^{-3}
DK	K_d - linear sorption distribution coefficient, L^3M^{-1}
EKF	K_f - Freundlich sorption coefficient, units depend on XNF
XNF	n - Freundlich sorption exponent, dimensionless
EKL	K_ℓ - Langmuir sorption coefficient, L^3M^{-1}
CEC	Q - Maximum sorption capacity or ion-exchange capacity, MM^{-1}
EK	K_m - Ion-exchange selectivity coefficient, dimensionless
CTOT	C_0 - Total solution concentration of two exchanging ions, equivalents/L^3

☆U.S. Government Printing Office: 1989-234-293

Errata

Modification of a method-of-characteristics solute-transport model to incorporate decay and equilibrium-controlled sorption or ion exchange

by D. J. Goode and L. F. Konikow, 1989, U.S. Geological Survey Water-Resources Investigations Report 89-4030, 65 p.

p. 10: Equations (17) and (18) should read:

$$\frac{d\bar{C}}{dC}=\frac{K_\ell Q}{(1+K_\ell C)^2}\;. \tag{17}$$

$$R_f(C)=1+\frac{\rho_b}{\varepsilon}\left[\frac{K_\ell Q}{(1+K_\ell C)^2}\right]\;. \tag{18}$$

The computer program statements listed in the report are consistent with these corrected equations.

p. 10: The fourth line of text from the bottom should read:
"The ion-exchange selectivity coefficient, K_m (units depend on stoichiometry), for this reaction is"

p. 10: The following sentence should be inserted after equation (20):
"If m = n, the exponents in eq. 20 are removed, or set to one."

p. 21: The fifth line of text from the bottom of the page should read:
"$\partial C/\partial x=0$, which approximates the boundary condition for the analytical"

p. 22: Table 1, the fourth line in the table should read:
"Bulk density of porous medium $\rho_b = 1.587$ g/cm^3 "

p. 30: The fourth line from the bottom of the page should read:
"advective flux only, $\partial C/\partial x = 0$ at x = -220 m and x = 673.33 m, and no transport,"

p. 31: Table 2, the ninth line in the table should read:
"Bulk density of porous medium $\rho_b = 2.16$ g/cm^3 "

p. 33 and 34: The text "analytic solution (solid line)," should be removed from the captions for Figures 12 and 13.

p. 65: The fifteenth line of text from the bottom of the page should read:
"5 divalent exchange RHOB, EK, CEC, CTOT, THALF"

p. 65: The third line of text from the bottom of the page should read:
"EK K_m - Ion-exchange selectivity coefficient, units depend on stoichiometry"

20 July 1989 (date of preceding errata)