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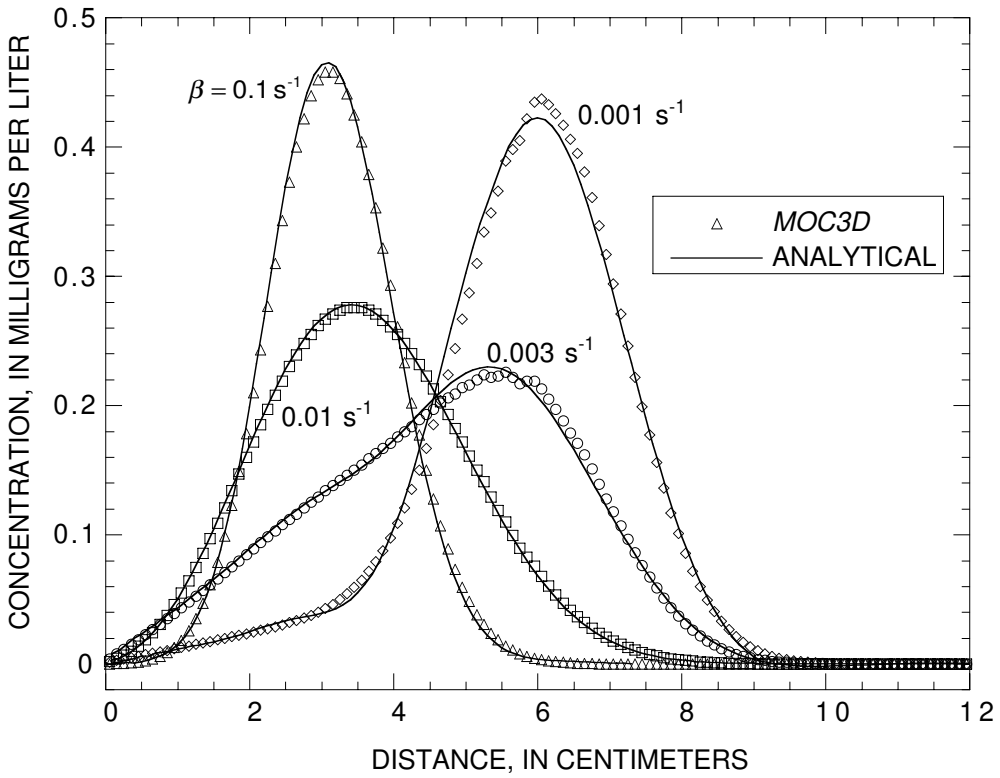
Age, Double Porosity, and Simple Reaction Modifications for the MOC3D Ground-Water Transport Model

Water-Resources Investigations Report 99-4041



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Cover: Numerical (MOC3D version 3.0) and analytical solutions for several different cases for solute transport in a one-dimensional, steady flow field with double porosity (see figure 3 of this report and related discussion). The variable is the linear exchange coefficient, β. Double-porosity parameters are listed in table 6 and other parameters are listed in table 5. [Abbreviation: s^{-1}, per second]

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by Daniel J. Goode

Water-Resources Investigations Report 99-4041

Lemoyne, Pennsylvania
1999

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PREFACE

This report describes modifications to a three-dimensional solute-transport model *(MOC3D)* developed by the U.S. Geological Survey (USGS). These modifications expand the capabilities of *MOC3D* to simulate (a) age of water in an aquifer; (b) effects of double porosity on concentrations of a single solute, and (c) effects of decay and zero-order growth reactions on a single solute. These modifications are incorporated into *MOC3D* version 3.0.

Although extensive testing of *MOC3D* indicates that this model will yield reliable calculations for a wide variety of field problems, the user is cautioned that the accuracy and efficiency of the model can be appreciably affected for certain combinations of values for parameters and boundary conditions.

The code for *MOC3D* is available for downloading over the Internet from a USGS software repository. The repository is accessible from the USGS Water Resources Information web page at URL **http://water.usgs.gov/**. The public anonymous FTP site is on the Water Resources Information server (water.usgs.gov or 130.11.50.175) in the /pub/software directory. As the model code is revised or updated, new versions or releases will be made available for downloading from these repositories.

CONTENTS

Page

ABSTRACT 1
INTRODUCTION 2
THEORETICAL BACKGROUND AND GOVERNING EQUATIONS 3
Governing Equation for Solute Transport 3
Governing Equation for Ground-Water Age Transport 5
NUMERICAL METHODS 6
Solute-Transport Equation 6
Method of Characteristics 6
Decay 7
Node Concentrations 7
Finite-Difference Approximations 8
Explicit-Dispersion Method 9
Implicit-Dispersion Method 10
Ground-Water Age Transport Equation 11
COMPUTER PROGRAM 11
General Program Features 11
Program Segments 12
MODEL TESTING AND EVALUATION 13
Decay and Sorption in One-Dimensional Steady Flow 13
Zero-Order Loss in One-Dimensional Steady Flow 15
Double-Porosity Exchange in One-Dimensional Steady Flow 16
Age in One-Dimensional Steady Flow 18
SUMMARY AND CONCLUSIONS 20
REFERENCES CITED 21
APPENDIX A
DATA INPUT INSTRUCTIONS FOR AGE, DOUBLE POROSITY, AND SIMPLE REACTIONS IN *MOC3D* 23
MOC3D Transport Name File (CONC) 23
AGE Input File 24
Double Porosity (DP) Input File 24
Simple Reactions (DK) Input File 25
APPENDIX B
ANNOTATED EXAMPLE INPUT DATASET FOR SAMPLE PROBLEM 27
APPENDIX C
SELECTED OUTPUT FOR SAMPLE PROBLEM 30

ILLUSTRATIONS

Page

1–4. Graphs showing:

1. Numerical *(MOC3D)* and analytical solutions for several different cases for solute transport in a one-dimensional, steady flow field with decay 15
2. Numerical *(MOC3D)* and analytical solutions for several different cases for solute transport in a one-dimensional, steady flow field with zero-order loss and no dispersion 16
3. Numerical *(MOC3D)* and analytical solutions for several different cases for solute transport in a one-dimensional, steady flow field with double porosity 18
4. Numerical *(MOC3D)* and analytical solutions for ground-water age transport in a one-dimensional, steady flow field with no dispersion 20

TABLES

1. Primary *MOC3D* 3.0 subroutine files modified for age, double porosity, and simple reactions 12
2. *MOC3D* 3.0 subroutines for AGE 12
3. *MOC3D* 3.0 subroutines for Double Porosity (DP) 13
4. *MOC3D* 3.0 subroutines for Simple Reactions (DK) 13
5. Parameters used in *MOC3D* simulation of transport in a one-dimensional, steady-state flow system 14
6. Modified and additional *MOC3D* parameters for double-porosity simulation 17

Age, Double Porosity, and Simple Reaction Modifications for the *MOC3D* Ground-Water Transport Model

Daniel J. Goode

ABSTRACT

This report documents modifications for the *MOC3D* ground-water transport model to simulate (a) ground-water age transport; (b) double-porosity exchange; and (c) simple but flexible retardation, decay, and zero-order growth reactions. These modifications are incorporated in *MOC3D* version 3.0. *MOC3D* simulates the transport of a single solute using the method-of-characteristics numerical procedure. The age of ground water, that is the time since recharge to the saturated zone, can be simulated using the transport model with an additional source term of unit strength, corresponding to the rate of aging. The output concentrations of the model are in this case the ages at all locations in the model. Double porosity generally refers to a separate immobile-water phase within the aquifer that does not contribute to ground-water flow but can affect solute transport through diffusive exchange. The solute mass exchange rate between the flowing water in the aquifer and the immobile-water phase is the product of the concentration difference between the two phases and a linear exchange coefficient. Conceptually, double porosity can approximate the effects of dead-end pores in a granular porous media, or matrix diffusion in a fractured-rock aquifer. Options are provided for decay and zero-order growth reactions within the immobile-water phase. The simple reaction terms here extend the original model, which included decay and retardation. With these extensions, (a) the retardation factor can vary spatially within each model layer, (b) the decay rate coefficient can vary spatially within each model layer and can be different for the dissolved and sorbed phases, and (c) a zero-order growth reaction is added that can vary spatially and can be different in the dissolved and sorbed phases. The decay and growth reaction terms also can change in time to account for changing geochemical conditions during transport. The report includes a description of the theoretical basis of the model, a detailed description of input requirements and output options, and the results of model testing and evaluation. The model tests illustrate use of these modifications and demonstrate that accurate solutions can be obtained for these simple cases. Two test cases have no dispersion, illustrating the suitability of this method-of-characteristics model for simulation of advection-dominated transport in ground water.

INTRODUCTION

Konikow and others (1996) describe *MOC3D*, a general purpose three-dimensional numerical model of solute transport in ground water. *MOC3D* functions as a package in *MODFLOW* (Harbaugh and McDonald, 1996) and uses fluxes and other flow information computed by *MODFLOW*. *MOC3D* can be applied to a wide variety of field problems. However, the user should first become aware of the assumptions and limitations inherent in the model, as described by Konikow and others (1996). *MOC3D* is a general tool that is applicable to a wide range of field problems involving solute transport. However, the model results could be inaccurate or model operation inefficient in some situations. Konikow and others (1996) provide guidelines for recognizing and avoiding these types of problems. Kipp and others (1998) add the capability to solve the dispersion and fluid-source parts of the transport equation implicitly to *MOC3D* (version 2).

The types of reactions incorporated into versions 1 and 2 of *MOC3D* are restricted to those that can be represented by a first-order rate reaction, such as radioactive decay, and those that can be represented by a retardation factor, such as instantaneous, reversible, sorption-desorption governed by a linear isotherm and constant distribution coefficient *(K_d)*. The retardation factor is assumed to be uniform in each model layer, and the decay coefficient is assumed to be uniform throughout the entire model domain. Furthermore, decay is assumed to occur at the same rate in the dissolved and sorbed phases, as would be the case for radioactive decay.

In this report, modifications for *MOC3D* that provide flexibility in approximating concentration changes due to geochemical reactions are presented. The retardation factor is modified so that it can vary spatially throughout the model domain, cell by cell, rather than layer by layer. This may allow simulations that approximate spatial changes in sorption coefficients due to spatial variability in aquifer composition or geochemistry. The decay coefficient also is modified so that it can vary spatially in three dimensions. Furthermore, separate decay coefficients may be used for the dissolved and sorbed phases. This modification may allow a more accurate approximation of biodegradation of organics, in which the degradation rate may be substantially different in the sorbed and dissolved phases. A new reaction, a zero-order growth reaction, is added in this version (3.0) of *MOC3D*. Zero-order loss can be simulated by use of a negative growth rate. The zero-order growth rate can vary spatially in three dimensions in the model domain. Finally, the decay coefficients and the zero-order growth rates can change in time; new values are optionally read at the beginning of each *MODFLOW* flow-model stress period (Harbaugh and McDonald, 1996).

This report also documents modifications to *MOC3D* for simulation of ground-water age (Goode, 1996, 1998) and double porosity. The ground-water age, defined as the time since recharge to the saturated zone, can be directly simulated by use of a solute-transport equation with a zero-order source term of unit strength. The output concentrations in this case are the volume-weighted-average ages. Double porosity generally refers to an immobile-water phase that does not contribute to ground-water flow but may affect solute concentrations by diffusive exchange. This conceptual model can approximate the effects of dead-end pores in granular porous media or of a low-permeability rock matrix in a fractured-rock aquifer. The double-porosity model is compatible with age transport, but decay and zero-order growth reactions are not compatible with age transport.

This report, in conjunction with the reports describing versions 1 (Konikow and

others, 1996) and 2 (Kipp and others, 1998), fully documents version 3.0 of *MOC3D*. The report includes a description of the numerical methods used to solve the solute-transport equation. The data requirements, input format specifications, program options, and output formats are all structured in a general manner that should be compatible with the types of data available for many field problems. The computer code is written in FORTRAN and has been developed in a modular style, similar to the *MODFLOW* model. Where possible, these modifications use available *MOC3D* modules and *MODFLOW* output modules.

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THEORETICAL BACKGROUND AND GOVERNING EQUATIONS

Mathematical equations that describe ground-water flow and transport processes may be developed from the fundamental principle of conservation of mass of water or of solute. A statement of conservation of mass (or continuity equation) may be combined with a mathematical description of the relevant process to obtain a differential equation describing flow or transport (see, for example, Bear, 1979; Freeze and Cherry, 1979; Domenico and Schwartz, 1990). Transport equations are presented here for two cases: solute transport and ground-water age transport.

Governing Equation for Solute Transport

The principle of conservation of mass requires that the net mass of solute entering and leaving a specified volume of aquifer during a given time interval must equal the accumulation or loss of mass stored in that volume during the interval. This relation may be expressed mathematically in a general governing equation for solute transport in three dimensions in an incompressible fluid flowing through a porous medium as (Bear, 1979, p. 239-243; Goode and Konikow, 1989; Konikow and others, 1996)

$$\frac{\partial(\varepsilon C)}{\partial t}+\frac{\partial(\rho_b \overline{C})}{\partial t}+\frac{\partial}{\partial x_i}\left(\varepsilon C V_i\right) - \frac{\partial}{\partial x_i}\left(\varepsilon D_{ij}\frac{\partial C}{\partial x_j}\right)-\sum C' W + \lambda\varepsilon C+\overline{\lambda}\rho_b \overline{C}-\Sigma=0 \quad , \qquad (1)$$

where ε is porosity, C is volumetric concentration (mass of solute per unit volume of water, ML^{-3}), ρ_b is the bulk density of the aquifer material (mass of solids per unit volume of aquifer, ML^{-3}), $\overline{C}$ is the mass concentration of solute sorbed on or contained within the solid aquifer material (mass of solute per unit mass of aquifer material, MM^{-1}), $\boldsymbol{V}$ is a vector of interstitial water velocity components (LT^{-1}), $\boldsymbol{D}$ is a second-rank tensor of dispersion coefficients (L^2T^{-1}), W is a volumetric water sink ($W<0$) or water source ($W>0$) rate per unit volume of aquifer (T^{-1}), C' is the volumetric concentration in the sink/source water (ML^{-3}), λ is the decay rate (T^{-1}) for the dissolved phase, $\overline{\lambda}$ is the decay rate for the sorbed phase, and Σ is a source or growth rate per unit aquifer volume ($ML^{-3}T^{-1}$).

The decay terms in equation 1 often represent radioactive decay of the free and sorbed solute. A radioactive decay rate is usually expressed as a half-life ($t_{1/2}$). The half-life is the time required for the concentration to decrease to one-half of the original value and is related to the decay rate as

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

In the case of radioactive decay, the decay rate is the same for all phases. In limited cases, the decay term also can adequately represent chemical decomposition or biodegradation (Bekins and others, 1998). However, if a

sorbed phase also is present in these latter cases, the decay process may occur at different rates in the dissolved and sorbed phases. A negative decay rate corresponds to first-order growth; in this case, the doubling time (t_{2X}) is given by

$$t_{2X} = \frac{(\ln 2)}{-\lambda} \quad . \tag{3}$$

The source term Σ is further defined to include zero-order growth in either the dissolved or sorbed phases, as well as exchange with an immobile phase. The zero-order source terms represent internal production of the solute without water and are characterized by mass production or growth rates. For the case of production in the water, $\Sigma = \varepsilon Z$, where Z is a zero-order growth rate per unit water volume ($ML^{-3}T^{-1}$) for the dissolved phase. Likewise, for production in the sorbed phases, $\Sigma = \rho_b Z'$, where $\overline{Z}'$ is the zero-order growth rate per unit rock mass ($MM^{-1}L^{-1}$) for the sorbed phase. Negative values of Z and $\overline{Z}'$ correspond to zero-order loss and may be applicable for some cases of biodegradation (Bekins and others, 1998). Such zero-order loss coefficients are nonlinear in that their values become zero when the solute concentration drops to zero.

Another internal source accounts for exchange between the water in the aquifer and a separate mass of immobile water. An approximate linear exchange model is assumed here such that the mass flux rate is the product of a linear exchange coefficient, β (T^{-1}), and the concentration difference between the immobile water and the flowing water:

$$\Sigma = \beta\left(\tilde{C} - C\right) , \tag{4}$$

where $\tilde{C}$ is the concentration in the immobile-water phase. This immobile water can conceptually correspond to dead-end pores in a granular aquifer (Coats and Smith, 1964) or to matrix diffusion in a fractured-rock aquifer (Bibby, 1981). Furthermore, this mathematical form is identical to that used to model kinetic sorption (Valocchi, 1985), provided the adsorption and desorption rate coefficients are equal. The double-porosity model can also simulate certain solute sources. The linear exchange coefficient may correspond to the dissolution rate coefficient of a separate-phase source. An artificially high linear exchange coefficient and porosity will cause the concentration in the mobile phase to be essentially fixed at $\tilde{C}$.

Combining these separate source terms and substituting into equation 1, the governing equation becomes

$$\frac{\partial(\varepsilon C)}{\partial t} + \frac{\partial(\rho_b \overline{C})}{\partial t} + \frac{\partial}{\partial x_i}\left(\varepsilon C V_i\right) - \sum C' W - \frac{\partial}{\partial x_i}\left(\varepsilon D_{ij} \frac{\partial C}{\partial x_j}\right) + \lambda \varepsilon C + \overline{\lambda} \rho_b \overline{C} - \varepsilon Z - \rho_b \overline{Z}' - \beta\left(\tilde{C} - C\right) = 0 \quad . \tag{5}$$

The governing equation for mass conservation in the immobile-water phase is

$$\tilde{\varepsilon} \frac{d\tilde{C}}{dt} + \tilde{\lambda} \tilde{\varepsilon} \tilde{C} - \tilde{\varepsilon} \tilde{Z} + \beta\left(\tilde{C} - C\right) = 0 \quad , \tag{6}$$

where $\tilde{\varepsilon}$ is the porosity, $\tilde{\lambda}$ is the decay rate (T^{-1}), and $\tilde{Z}$ is the zero-order growth rate ($ML^{-3}T^{-1}$), each for the immobile-water phase.

A simpler "flow-equation-removed" form of the governing equation is derived by removing velocity divergence terms, $\partial(\varepsilon V_i)/\partial x_i$ (Konikow and Grove, 1977; Goode, 1990, 1992; Konikow and others, 1996), leaving

$$\frac{\partial C}{\partial t} + \frac{\partial(\rho_b \overline{C})}{\varepsilon \partial t} + V_i \frac{\partial C}{\partial x_i} - \frac{\frac{\partial}{\partial x_i}\left(\varepsilon D_{ij} \frac{\partial C}{\partial x_j}\right)}{\varepsilon} - \frac{\Sigma\left[W(C' - C)\right]}{\varepsilon} + \lambda C + \frac{\rho_b \overline{\lambda}\, \overline{C}}{\varepsilon} - Z - \frac{\rho_b \overline{Z}'}{\varepsilon} - \frac{\beta}{\varepsilon}\left(\tilde{C} - C\right) = 0 \quad . \tag{7}$$

The governing equation can be further simplified for the case of reversible, instantaneous, equilibrium sorption of the solute governed by a linear isotherm. For this case, the sorbed concentration, $\overline{C}$, is given by

$$\overline{C} = K_d C \quad , \tag{8}$$

where K_d is the sorption coefficient, or distribution coefficient, which is assumed to be constant in time. The accumulation in the sorbed phase can be expressed as

$$\frac{\partial(\rho_b \overline{C})}{\partial t} = K_d \frac{\partial(\rho_b C)}{\partial t} = \rho_b K_d \frac{\partial C}{\partial t} \quad , \tag{9}$$

if it is assumed that the aquifer bulk density is constant in time. Substituting equations 8 and 9 into equation 7 gives

$$\left(1 + \frac{\rho_b K_d}{\varepsilon}\right)\frac{\partial C}{\partial t} + V_i \frac{\partial C}{\partial x_i} - \frac{\frac{\partial}{\partial x_i}\left(\varepsilon D_{ij} \frac{\partial C}{\partial x_j}\right)}{\varepsilon} - \frac{\Sigma\left[W(C' - C)\right]}{\varepsilon} + C\left(\lambda + \frac{\rho_b K_d \overline{\lambda}}{\varepsilon}\right) - Z - \frac{\rho_b \overline{Z}'}{\varepsilon} - \frac{\beta}{\varepsilon}\left(\tilde{C} - C\right) = 0 \quad . \tag{10}$$

The terms controlling sorption can be combined into a single parameter, the retardation factor (R_f), which is defined as

$$R_f = 1 + \frac{\rho_b K_d}{\varepsilon} \quad . \tag{11}$$

R_f may vary slightly in time if the porosity changes due to transient flow effects. This possible slight variability is ignored and the retardation factor is assumed to be constant in time. Substituting equation 11 into equation 10 yields

$$\frac{\partial C}{\partial t} + \frac{V_i}{R_f}\frac{\partial C}{\partial x_i} - \frac{1}{\varepsilon R_f}\frac{\partial}{\partial x_i}\left(\varepsilon D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\Sigma\left[W(C' - C)\right]}{\varepsilon R_f} + \frac{C}{R_f}\left[\lambda + \left(R_f - 1\right)\overline{\lambda}\right] - \frac{Z}{R_f} - \frac{\left(R_f - 1\right)\overline{Z}}{R_f} - \frac{\beta}{\varepsilon R_f}\left(\tilde{C} - C\right) = 0 \quad , \tag{12}$$

where $\overline{Z} = \overline{Z}' / K_d$. The growth term for the sorbed phase is in terms of an equivalent dissolved-phase rate. This is the form of the governing equation solved in this version (3.0) of *MOC3D*. This governing equation is coupled to the immobile-water phase governing equation 6 through the exchange term $\beta\left(\tilde{C} - C\right)$.

Converting equation 12 from an Eulerian to a Lagrangian framework through the material derivative yields a simpler form of the governing equation (for example, see Konikow and Bredehoeft, 1978, p. 6) for the concentration of a reference point moving with the retarded velocity (V/R_f)

$$\frac{\mathrm{d}C}{\mathrm{d}t} - \frac{1}{\varepsilon R_f}\frac{\partial}{\partial x_i}\left(\varepsilon D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\Sigma\left[W(C' - C)\right]}{\varepsilon R_f} + \frac{C}{R_f}\left[\lambda + \left(R_f - 1\right)\overline{\lambda}\right] - \frac{Z}{R_f} - \frac{\left(R_f - 1\right)\overline{Z}}{R_f} - \frac{\beta}{\varepsilon R_f}\left(\tilde{C} - C\right) = 0 \quad . \tag{13}$$

Although this concentration is now that of a moving point in space, the same symbol, C, is retained for convenience.

Boundary and initial conditions, and internal sources associated with water sources, are described by Konikow and others (1996).

Governing Equation for Ground-Water Age Transport

A special form of the solute transport equation can be used to simulate ground-water

age transport. Dropping the decay and sorption reactions from the governing equation 12 developed above leaves a governing equation that includes zero-order growth in the dissolved phase and double-porosity exchange:

$$\frac{\partial C}{\partial t} + V_i \frac{\partial C}{\partial x_i} - \frac{\frac{\partial}{\partial x_i}\left(\varepsilon D_{ij} \frac{\partial C}{\partial x_j}\right)}{\varepsilon} - \frac{\Sigma\left[W\left(C' - C\right)\right]}{\varepsilon} - Z - \frac{\beta}{\varepsilon}\left(\tilde{C} - C\right) = 0 \quad . \tag{14}$$

Ground-water age can be simulated by an advection-dispersion transport equation of the form (Goode, 1996, 1998)

$$\frac{\partial A}{\partial t} + V_i \frac{\partial A}{\partial x_i} - \frac{\frac{\partial}{\partial x_i}\left(\varepsilon D_{ij} \frac{\partial A}{\partial x_j}\right)}{\varepsilon} - \frac{\Sigma\left[W\left(A' - A\right)\right]}{\varepsilon} - 1 - \frac{\beta}{\varepsilon}\left(\tilde{A} - A\right) = 0 \quad , \tag{15}$$

where A (T) is the volume-average ground-water age in the aquifer, or time since recharge; A' (T) is the age of water in external sources, and $\tilde{A}$ (T) is the age of water in the immobile-water phase. By examination, the age-transport equation is identical to the solute-transport equation under the following conditions:

- all concentrations are replaced with corresponding ages
- the zero-order growth rate has unit (1) value, and
- decay and sorption reactions are not present.

The most common application of this equation is for steady-state conditions in which the time derivative term is zero. A steady-state solution does not exist if both ***V*** and ***D*** are zero.

Boundary and initial conditions for age-transport simulation based on equation 15 are consistent with the normal form of the solute-transport equation (Goode, 1996). In general, the age of incoming water is zero, but non-zero values can be specified as appropriate. The standard 'natural' outflow condition implies that age is carried out of the aquifer with discharging water and no dispersion occurs across boundaries. The initial age of water in the aquifer and in the immobile-water phase, if present, must be specified. At very large times, the solution is not sensitive to the initial condition, but it is mathematically required.

The numerical methods described below are given in terms of solute concentrations. These same methods are used for the age-transport equation. In this case, the particle and node concentrations are particle and node ages. Furthermore, the decay and growth reaction terms are not used for the age-transport numerical solution.

NUMERICAL METHODS

The notation and conventions used in this report and in the *MOC3D* version 3.0 code to describe the grid and to reference (or to number) nodes are described by Konikow and others (1996). The indexing notation used here is consistent with that used in the FORTRAN code for *MODFLOW* by McDonald and Harbaugh (1988), although not necessarily the notation used in the text of their report.

Solute-Transport Equation

Method of Characteristics

As described by Konikow and others (1996), the advective part of the transport solution is computed by a system of moving particles that track 'retarded' solute motion in the aquifer. The remaining processes affecting

concentrations are left in a partial differential equation describing the concentrations of those moving particles. Equation 13 can be rearranged to express the temporal change in concentration as

$$\frac{\mathrm{d}C}{\mathrm{d}t} = \frac{1}{\varepsilon R_f}\frac{\partial}{\partial x_i}\left(\varepsilon D_{ij}\frac{\partial C}{\partial x_j}\right) + \frac{\Sigma\left[W(C'-C)\right]}{\varepsilon R_f} - \frac{C}{R_f}\left[\lambda + \left(R_f - 1\right)\bar{\lambda}\right] + \frac{Z}{R_f} + \frac{\left(R_f - 1\right)\bar{Z}}{R_f} + \frac{\beta}{\varepsilon R_f}\left(\tilde{C} - C\right) . \quad (16)$$

Integration of the transport problem for one transport time step involves first moving particles to new locations and then adjusting particle concentrations according to equation 16 (Konikow and others, 1996). The approach taken to couple advection and other transport processes is to compute node concentrations on a finite-difference grid from the particle concentrations, and use these node concentrations to compute the concentration gradients and changes in equation 16. These computed concentration changes are then applied to individual particles, and the time-step cycle is complete.

Decay

Decay is simulated by reducing the particle concentrations during advection. During the advective step, the particle concentration has not yet been adjusted for dispersion and sources. However, the change in particle position accounts for advection up to time increment $t+\Delta t$. An analytical solution for concentration during decay, ignoring all other processes, is used to compute new particle concentrations after decay. The loss of solute mass during a given transport time increment (Δt) because of decay processes is accounted for by computing the decayed particle concentration, C_p^d, as

$$C_p^d = C_p^t \; e^{-\lambda_{eff}\Delta t} \quad , \quad (17)$$

where $\lambda_{eff} = \frac{1}{R_f}\left[\lambda + \left(R_f - 1\right)\bar{\lambda}\right]$

is an effective decay rate and C_p^t is the particle concentration at the start of the move interval (and before advection). All terms in equation 17 are evaluated for the finite-difference cell where the particle is located after moving, at the end of the transport time step. If $R_f = 1$ (no retardation), or if $\bar{\lambda} = \lambda$, the effective decay rate is simply λ.

As noted by Goode and Konikow (1989), the exponential formulation of equation 17 has no associated numerical stability restrictions. However, if the half-life is on the order of the transport time increment or smaller, some accuracy will be lost because of the explicit de-coupling of decay and other transport processes.

Node Concentrations

After all particles have been moved, the concentration at each node is temporarily assigned the average concentration of all particles then located within the volume of that cell; this average concentration is denoted as $C_{j,i,k}^{adv}$:

$$C_{j,i,k}^{adv} = \frac{\sum_{p=1}^{N} C_p^d \delta\left(j_p^{t+1} = j, i_p^{t+1} = i, k_p^{t+1} = k\right)}{\sum_{p=1}^{N} \delta\left(j_p^{t+1} = j, i_p^{t+1} = i, k_p^{t+1} = k\right)} , \quad (18)$$

where the δ function is 1 if the particle is within the cell *j,i,k* and is zero otherwise. The time index is labeled "*adv*" because this temporarily assigned average concentration represents the new time level only with respect to advective transport and decay. With respect to the finite-difference grid, the effect of advective transport is to move particles with differing concentrations into and out of each cell.

Finite-Difference Approximations

The divergence of dispersive flux is normalized by the retardation factor and porosity to yield the rate of change in concentration. In addition, in a quasi-3D approach, changes in saturated thickness are incorporated for horizontal flux terms. Standard finite-difference methods are applied to the governing partial differential equation. Hence, derivatives in the governing equation are approximated by differences. For the time derivative, the rate of change in time is approximated by the difference between concentrations at two time levels divided by the transport time increment. Similarly, the spatial derivatives are replaced by differences between adjacent nodes (cell centers) in the finite-difference grid. The rate of change in concentration due to dispersion, water sources, zero-order sources, and exchange with an immobile-water phase can be written as (after Konikow and others, 1996)

$$\frac{C_{j,i,k}^{t+1}-C_{j,i,k}^{t}}{\Delta t}=\frac{1}{\left(R_f\right)_{j,i,k}\left(\varepsilon b\right)_{j,i,k}^{t+1}}\left\{\Delta x^{-1}\left[\left(\varepsilon b D_{1m}\frac{\partial C}{\partial x_m}\right)_{j+1/2,i,k}^{*}-\left(\varepsilon b D_{1m}\frac{\partial C}{\partial x_m}\right)_{j-1/2,i,k}^{*}\right]\right.$$
$$+\Delta y^{-1}\left[\left(\varepsilon b D_{2m}\frac{\partial C}{\partial x_m}\right)_{j,i+1/2,k}^{*}-\left(\varepsilon b D_{2m}\frac{\partial C}{\partial x_m}\right)_{j,i-1/2,k}^{*}\right]$$
$$\left.+\left[\left(\varepsilon D_{3m}\frac{\partial C}{\partial x_m}\right)_{j,i,k+1/2}^{*}-\left(\varepsilon D_{3m}\frac{\partial C}{\partial x_m}\right)_{j,i,k-1/2}^{*}\right]+\sum_{W>0}\left[W_{j,i,k}\left(C'_{j,i,k}-C_{j,i,k}^{*}\right)\right]\right\}$$
$$+\left(R_f\right)_{j,i,k}^{-1}\left\{Z_{j,i,k}+\left[\left(R_f\right)_{j,i,k}-1\right]\overline{Z}_{j,i,k}+\frac{\beta_{j,i,k}}{\varepsilon_{j,i,k}^{t+1}}\left(\tilde{C}_{j,i,k}-C_{j,i,k}^{*}\right)\right\}\quad , \qquad (19)$$

where subscript *m* is a summation index for the dispersion term. The *j,i,k* subscripts in equation 19 denote the spatial finite-difference grid indexing, as described by Konikow and others (1996). The superscript "*" indicates that the terms depend on the average of the concentration at the old time level and the concentration at the new time level after advection and decay:

$$C_{j,i,k}^{*}=\frac{C_{j,i,k}^{t}+C_{j,i,k}^{adv}}{2}\ . \qquad (20)$$

These averaged concentrations are used to calculate the solute flux terms indicated by the superscript "*."

The components of the dispersive flux in each direction across cell faces are calculated by use of centered-in-space finite-difference approximations. A detailed description of these finite-difference approximations is given by Konikow and others (1996).

In the method-of-characteristics approach, the change in concentration during each transport time increment is computed for each cell in the model, and then that change in concentration is applied to each particle within that cell at the end of the time increment. Version 3.0 of *MOC3D* documented in this report has two optional methods for computing that change in cell concentration during a time increment: a fully explicit method (Konikow

and others, 1996) and an implicit method (Kipp and others, 1998). These methods retain an explicit de-coupling of advection and decay from the other transport processes affecting concentrations. Incorporation of the modified and added reaction terms in these alternate methods are described below.

The procedure to change particle concentrations depends on the sign of the total change in concentration (Konikow and others, 1996). For a positive change, or increasing concentrations, the change in concentration is added to all particles located in the cell. If the concentration change is negative, the ratio of the new concentration to the old concentration is used to scale all particle concentrations, resulting in proportional changes in individual particle concentrations.

Explicit-Dispersion Method

Following Konikow and others (1996), all terms on the right-hand side of equation 19 are evaluated by use of known concentrations in the flowing water, C^*, which is the average of the concentration at the previous time level and the concentration at the new time level after advection and decay only. The only other unknown is the concentration in the immobile-water phase, $\tilde{C}$. This concentration is computed first at the new time level by use of a centered-in-time finite-difference method.

A centered-in-time finite-difference approximation for the concentration in the immobile-water phase can be written (in this and following equations, the node index *j,i,k* is implicit for all terms)

$$\frac{\tilde{C}^{t+1}-\tilde{C}^{t}}{\Delta t}=\tilde{Z}-\frac{\tilde{\lambda}}{2}\left(\tilde{C}^{t+1}+\tilde{C}^{t}\right)+\frac{\beta}{2\tilde{\varepsilon}}\left(2C^{*}-\tilde{C}^{t+1}-\tilde{C}^{t}\right) \quad . \qquad (21)$$

Grouping unknown terms at the new time level on the left-hand side gives

$$\tilde{C}^{t+1}\left(\frac{1}{\Delta t}+\frac{\tilde{\lambda}}{2}+\frac{\beta}{2\tilde{\varepsilon}}\right)=\frac{\tilde{C}^{t}}{\Delta t}+\tilde{Z}-\frac{\tilde{\lambda}}{2}\tilde{C}^{t}+\frac{\beta}{2\tilde{\varepsilon}}\left(2C^{*}-\tilde{C}^{t}\right) \quad , \qquad (22)$$

from which the concentration at the new time level is computed. The average of the new and old time level concentration is used to compute the mass flux to the flowing water phase.

The change in concentration due to dispersion and sources is computed as described by Konikow and others (1996), with the minor modification that the retardation factor is allowed to vary from cell to cell and is thus indexed by all three spatial indices, *j,i,k*.

The additional change in concentration due to zero-order sources and double-porosity exchange (ΔC) is

$$\Delta C=\frac{\Delta t}{R_f}\left[Z+\left(R_f-1\right)\overline{Z}+\frac{\beta}{2\varepsilon^{t+1}}\left(\tilde{C}^{t+1}+\tilde{C}^{t}-2C^{*}\right)\right]. \qquad (23)$$

Numerical mass conservation between the flowing and immobile-water phases is maintained by use of the same expression for exchange flux in both finite-difference expressions. This change in concentration is added to the concentration changes from dispersion and sources and used to modify cell and particle concentrations as described above (see Konikow and others, 1996).

For the case of explicit dispersion and source calculations, a new stability criterion is used for the double-porosity calculations. As with the stability criteria developed for sources (Konikow and others, 1996; Konikow and Bredehoeft, 1978), this criteria limits mass flux in one transport time step due to double-porosity exchange to total mass available in the cell. This condition can be expressed as

$$\frac{\Delta t\,\beta}{\varepsilon R_f} \le 1.0 \quad . \qquad (24)$$

Solving equation 24 for Δt at all nodes yields the criterion

$$\Delta t \le \underset{\text{(over grid)}}{\text{Min}} \left[\frac{\left(\varepsilon R_f\right)_{j,i,k}}{\beta_{j,i,k}} \right] . \qquad (25)$$

Because the exchange process with the immobile-water phase is occurring simultaneously with dispersion and injection, this new stability requirement is combined with dispersion and injection stability requirements. Thus, the limiting time-step size is determined from limiting by dispersion and double-porosity exchange, or by injection and double-porosity exchange, whichever is more restrictive. This stability limit is not needed for the implicit-dispersion method (Kipp and others, 1998). Hence, larger time steps can be taken using the implicit-dispersion method when dispersion or injection rates are high.

Implicit-Dispersion Method

Following Kipp and others (1998), all terms on the right-hand side of equation 19 are evaluated by use of a time-weighted average of old and new concentrations. The known concentration in the flowing water, C^*, is the average of the concentration at the previous time level and the concentration at the new time level after advection and decay only. Kipp and others (1998) describe the procedures to build an implicit matrix equation for concentrations at the new time level. The additional transport processes here affect only the diagonal matrix terms and the forcing vector on the right-hand side. Leaving out the dispersion and source terms already described by Kipp and others (1998), an implicit finite-difference equation for the change in concentration in the flowing water phase is

$$\delta C = \frac{\Delta t}{R_f}\left[Z + \left(R_f - 1\right)\overline{Z} + \frac{\beta}{2\varepsilon^{t+1}}\left(\tilde{C}^{t+1} + \tilde{C}^{t} - 2C^{*} - 2\theta\delta C \right) \right] , \qquad (26)$$

where θ is the implicit time-weighting coefficient. Fully-implicit integration for the flowing-water phase concentration corresponds to $\theta = 1$ and Crank-Nicolson (centered-in-time) integration corresponds to $\theta = 0.5$ (Kipp and others, 1998). The immobile-water concentration is unknown. However, this unknown term can be written in terms of only known concentrations and the new flowing-water concentration. Substituting this form into equation 24 yields an implicit equation in terms of the new concentration in the flowing water alone.

A centered-in-time finite-difference approximation for the concentration in the immobile-water phase can be written as

$$\frac{\tilde{C}^{t+1} - \tilde{C}^{t}}{\Delta t} = \tilde{Z} - \frac{\tilde{\lambda}}{2}\left(\tilde{C}^{t+1} + \tilde{C}^{t} \right) + \frac{\beta}{2\tilde{\varepsilon}}\left[2\left(C^{*} + \theta\delta C \right) - \tilde{C}^{t+1} - \tilde{C}^{t} \right] \quad . \qquad (27)$$

Grouping unknown terms at the new time level and rearranging results in

$$\tilde{C}^{t+1} = \frac{\beta\theta}{\tilde{\varepsilon}\left(\frac{1}{\Delta t} + \frac{\tilde{\lambda}}{2} + \frac{\beta}{2\tilde{\varepsilon}} \right)}\delta C + \left(\frac{1}{\Delta t} + \frac{\tilde{\lambda}}{2} + \frac{\beta}{2\tilde{\varepsilon}} \right)^{-1}\left[\frac{\tilde{C}^{t}}{\Delta t} + \tilde{Z} - \frac{\tilde{\lambda}}{2}\tilde{C}^{t} + \frac{\beta}{2\tilde{\varepsilon}}\left(2C^{*} - \tilde{C}^{t} \right) \right] \quad . \qquad (28)$$

The average of the new and old time level concentration is used to compute the mass flux to the flowing-water phase.

The equation for the immobile-phase concentration can be directly substituted into

the finite-difference equation for the mobile phase to yield a single implicit equation. The right-hand side of equation 28 is substituted into equation 26 and rearranged, yielding

$$\delta C = \left\{ \frac{\beta\theta\Delta t}{R_f \varepsilon^{t+1}} \left[\frac{\beta}{2\tilde{\varepsilon}} \left(\frac{1}{\Delta t} + \frac{\tilde{\lambda}}{2} + \frac{\beta}{2\tilde{\varepsilon}} \right)^{-1} - 1 \right] \right\} \delta C + \frac{\Delta t}{R_f} \left\{ Z + \left(R_f - 1 \right) \overline{Z} + \frac{\beta}{2\varepsilon^{t+1}} \left(\tilde{C}^t - 2C^* \right) \right.$$
$$\left. + \frac{\beta}{2\varepsilon^{t+1}} \left(\frac{1}{\Delta t} + \frac{\tilde{\lambda}}{2} + \frac{\beta}{2\tilde{\varepsilon}} \right)^{-1} \left[\tilde{Z} + \frac{\beta}{\tilde{\varepsilon}} C^* + \left(\frac{1}{\Delta t} - \frac{\tilde{\lambda}}{2} - \frac{\beta}{2\tilde{\varepsilon}} \right) \tilde{C}^t \right] \right. . \qquad (29)$$

The change in concentration due to dispersion and sources is computed as described by Kipp and others (1998), with the minor modification that the braced term in front of δC in equation 29 is subtracted from the diagonal coefficient of the conductance matrix. The remaining terms on the right-hand side of equation 29 are added to the forcing vector (**b** as defined by Kipp and others, 1998, p. 10).

After the concentration change for the flowing-water phase is computed implicitly, the concentration in the immobile-water phase is computed from equation 27. Numerical mass conservation between the flowing and immobile-water phases is maintained by use of the same expression for exchange flux in both finite-difference expressions.

Ground-Water Age Transport Equation

The ground-water age transport equation is solved by use of the numerical methods for the solute transport equation, as presented above, and by Konikow and others (1996) and Kipp and others (1998). In this context, the concentration of particles and nodes in the model corresponds to the age. Rather than compute the contribution of the zero-order source term (1) by use of the finite-difference grid, this term is added directly to particle ages in the age-transport model, similar to the methods used for decay in the solute-transport equation.

At the beginning of each transport time step, the age of each particle is increased by Δt, the length of the transport time step. Advection, dispersion, water source, and double-porosity processes are all simulated by use of the methods described here and in previous *MOC3D* documentation (Konikow and others, 1996; Kipp and others, 1998). Other than activating the age transport option, the only other input used is a conversion factor for the ages. By use of this conversion factor, the ages in the transport model can be in years even though the internal flow and transport model time unit is seconds, for example.

COMPUTER PROGRAM

General Program Features

The integration of the *MOC3D* transport program with the *MODFLOW* ground-water flow model is described by Konikow and others (1996) and Kipp and others (1998). Implementing *MOC3D* requires the use of a separate "name" file similar to the file used in *MODFLOW*. The principal *MOC3D* input data (such as subgrid dimensions, hydraulic properties, and particle information) are read from the main *MOC3D*

data file. Other files are used for observation wells, concentrations in recharge, and several input and output options. Three additional file types are used to activate the optional methods documented in this report. Detailed input data requirements and instructions for the *MOC3D* name file and for the new optional packages are presented in appendix A. Also, a sample input dataset for a test problem is included in appendix B.

MOC3D output is routed to a main listing file, separate from the *MODFLOW* listing file. Options are available for writing specific data to separate output files, which will facilitate graphical post-processing. Appendix C contains output from the sample dataset described in appendix B.

Program Segments

MOC3D and the modifications presented here are compatible with the version of *MODFLOW* designated as *MODFLOW-96* (Harbaugh and McDonald, 1996). The only changes to the flow-model programs are modification of the main routine to call subroutines for *MOC3D* and to pass necessary arrays and parameters for the optional methods presented here.

The primary MOC3D subroutines that are modified for the methods presented here are listed in table 1. One change made throughout the model is that the original array for layer-by-layer retardation factors has been expanded to a cell-by-cell array to accommodate the new spatially variable retardation factor option. This modification is transparent to the user.

The subroutines added to *MOC3D* for age, double porosity, and simple reactions are listed in tables 2, 3, and 4, respectively. The naming and function of these subroutines generally follows conventions used in *MODFLOW-96* and *MOC3D*.

Table 1. Primary *MOC3D* 3.0 subroutine files modified for age, double porosity, and simple reactions

Subroutine	Changes from version 2.0
MOC_MAIN6	Pass new variables and arrays to existing subroutines; Call new subroutines to compute changes in concentration for age, double porosity, and simple reactions
MOC6	Call new subroutines to read options and parameters for modifications
MOVE6	Age added, decay and retardation modified

Table 2. *MOC3D* 3.0 subroutines for AGE

Subroutine	Description
AGE6DF	Read time-unit conversion factor
AGE6AP	Add change in age for 1 transport time step to all particles and all nodes

Table 3. *MOC3D* 3.0 subroutines for Double Porosity (*DP*)

Subroutine	Description
DP6DF	Read double-porosity reaction and printing options
DP6AL	Allocate space in "X" array
DP6RP	Read parameters for double porosity
DP6AP	Solve double-porosity concentration equation for explicit-dispersion method
DP6IAP	Formulate double-porosity concentration equation for implicit-dispersion method
DP6IUP	Update double-porosity concentration for implicit-dispersion method
SDP6C	Print or save double-porosity concentrations
DP6MB	Double-porosity mass balance
DP6ST	Compute stability limits for double-porosity equation for explicit-dispersion method

Table 4. *MOC3D* 3.0 subroutines for Simple Reactions (*DK*)

Subroutine	Description
DK6DF	Read reaction options
DK6AL	Allocate space in "X" array
DK6RP	Read parameters for simple reactions
DK6DK	Compute effective decay rate coefficient for individual model cell
DK6AP	Compute changes in concentration due to zero-order growth reactions for explicit-dispersion method
DK6IAP	Add zero-order growth terms to conductance matrix and forcing vector for implicit-dispersion method
DK6MB	Reaction mass balance

MODEL TESTING AND EVALUATION

The results of the numerical model are compared to analytical solutions to illustrate the relative accuracy of the model and to provide examples of the model capabilities. Because of the idealized features of these problems, care should be taken in transferring the results of these tests to real-world problems. However, these results indicate that the model can accurately solve the ground-water transport equations described in this report with adequate spatial and temporal discretization. In addition to the tests discussed here, the test simulations described by Konikow and others (1996) have all been successfully re-run with version 3.0 of *MOC3D* utilizing the modified algorithms for retardation and decay. Tests of general solute-transport simulation capabilities of *MOC3D* are presented by Goode and Konikow (1991), Konikow and others (1996), and Kipp and others (1998). Hornberger and Konikow (1998) describe a graphical user-interface for *MOC3D*.

Decay and Sorption in One-Dimensional Steady Flow

Wexler (1992) presents an analytical solution for one-dimensional solute transport in a finite-length aquifer system having a third-type source boundary condition. The one-dimensional governing equation is

$$R_f \frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} - \lambda R_f C \quad . \qquad (30)$$

The governing equation is subject to the boundary conditions

$$VC' = VC - D\frac{\partial C}{\partial x}, \qquad x = 0 \qquad (31)$$

$$\text{and} \quad \frac{\partial C}{\partial x} = 0, \qquad x = L \qquad (32)$$

and initial condition

$$C = 0\ , \qquad 0 < x < L\ . \qquad (33)$$

For this and the following test problems, it is assumed that the length of the system, L, is equal to 12 cm, $C' = 1.0$, and $V = 0.1$ cm/s. The analytical solution is given by equations 52 and 53 of Wexler (1992, p. 17). The flow equation is solved by use of a one-dimensional grid having 122 cells (nodes) in the x direction. The solute-transport equation is solved in a 120-cell subgrid to assure a constant velocity within the transport domain and to allow an accurate match to the boundary conditions of the analytical solution. The grid spacing is $\Delta x = 0.1$ cm. The numerical solution is implemented by use of three initial particles per cell (NPTPND = 3) and a CELDIS factor of 0.5. The input parameters for the model simulation are summarized in table 5.

The effect of decay is evaluated by specifying the decay rate as $\lambda = 0.01$ s^{-1} without retardation (fig. 1), which agrees well with the analytical solution. Three different cases with a retardation factor of $R_f = 2$ and different values of decay coefficients for the dissolved and sorbed phases yield numerically identical solutions at $t = 180$ s. Decay is not reduced by the retardation effect, hence, these cases have effective decay rate coefficients that are one-half that of the base case without retardation. If retardation is included and the sorbed and dissolved phases decay at the same rate as the base case, concentrations are appreciably lower at $t = 180$ s. These results also agree well with the analytical solution.

Table 5. Parameters used in *MOC3D* simulation of transport in a one-dimensional, steady-state flow system.
[Abbreviations: cm^2/s, square centimeters per second; cm, centimeter; s, second; cm/s, centimeters per second]

Parameter	Value
$T_{xx} = T_{yy}$	0.01 cm^2/s
Porosity (ε)	0.1
Dispersivity (α_L)	0.1 cm
PERLEN (length of stress period)	90 or 180 s
Velocity (V_x)	0.1 cm/s
Initial concentration (C_0)	0.0
Source concentration (C')	1.0
Number of rows	1
Number of columns	122
Number of layers	1
DELR (Δx)	0.1 cm
DELC (Δy)	0.1 cm
Thickness (b)	1.0 cm
NPTPND (Initial number of particles per cell)	3
CELDIS	0.5
INTRPL (Interpolation scheme)	1

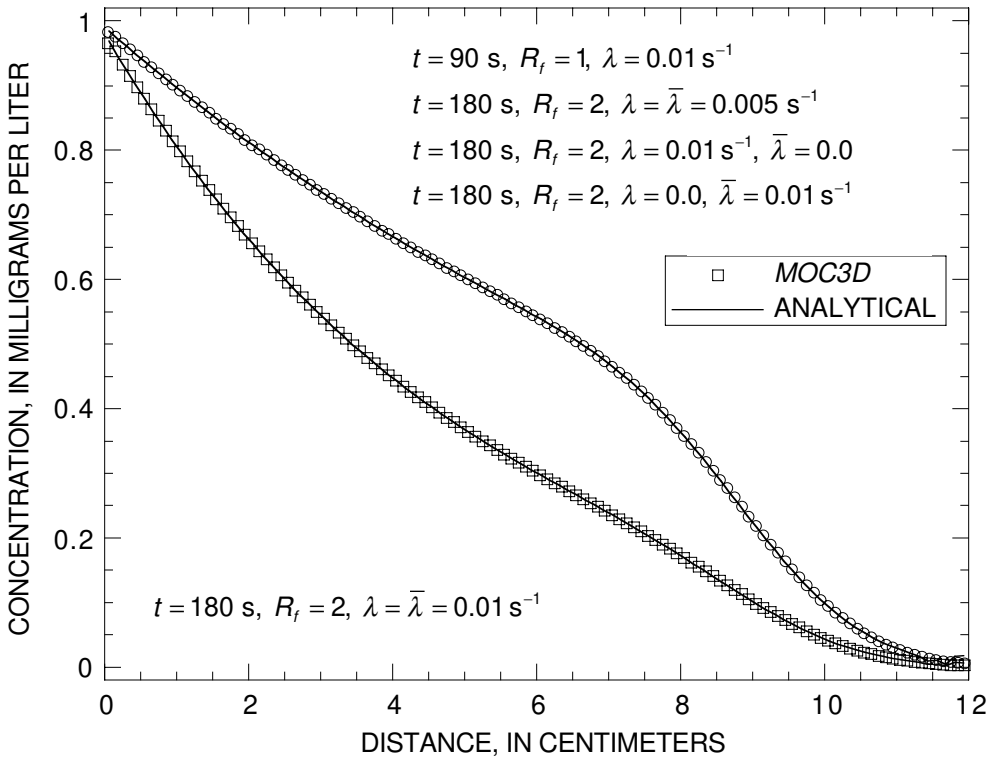

Figure 1. Numerical (*MOC3D*) and analytical solutions for five cases for solute transport in a one-dimensional, steady flow field with decay. Variables are time, *t,* retardation factor, R_f, dissolved phase decay rate coefficient, λ, and sorbed phase decay rate coefficient, $\bar{\lambda}$. Other parameters are listed in table 5. [Abbreviations: s, second; s^{-1}, per second]

Zero-Order Loss in One-Dimensional Steady Flow

The transport solution using the *DK* package with zero-order loss (negative growth) is tested by comparing the numerical solution to an analytical solution for a one-dimensional steady-flow case with no dispersion. The governing equation for this case is

$$\frac{\partial C}{\partial t} + \frac{V_i}{R_f}\frac{\partial C}{\partial x} - \frac{Z}{R_f} - \frac{\left(R_f - 1\right)\bar{Z}}{R_f} = 0. \qquad (34)$$

The equation is nonlinear when the growth terms are negative because they become zero if the concentration is zero. The hyperbolic governing equation is subject to the boundary condition

$$C = C_1, \qquad x = 0, \qquad (35)$$

and the initial condition

$$C = 0, \qquad 0 < x < L. \qquad (36)$$

The problem can be solved by use of coordinate transformations, yielding

$$C = H\left(\frac{Vt}{R_f} - x\right) H\left(\frac{C_1 V}{Z + \left(R_f - 1\right)\bar{Z}} - x\right) \left\{C_1 + \frac{x}{V}\left[Z + \left(R_f - 1\right)\bar{Z}\right]\right\}, \qquad (37)$$

where H is the Heaviside step function: $H(y) = 1$ for $y > 0$ and $H(y) = 0$ for $y \leq 0$. This

particular solution is for the case of negative Z and $\overline{Z}$, corresponding to zero-order loss. If the growth terms are positive, the second Heaviside function is removed.

The numerical model reproduces the analytical solution very closely for five cases with retardation and zero-order loss (fig. 2). A slight difference is noted at the advancing front, but this difference disappears as concentrations at the front drop to zero, numerically and analytically.

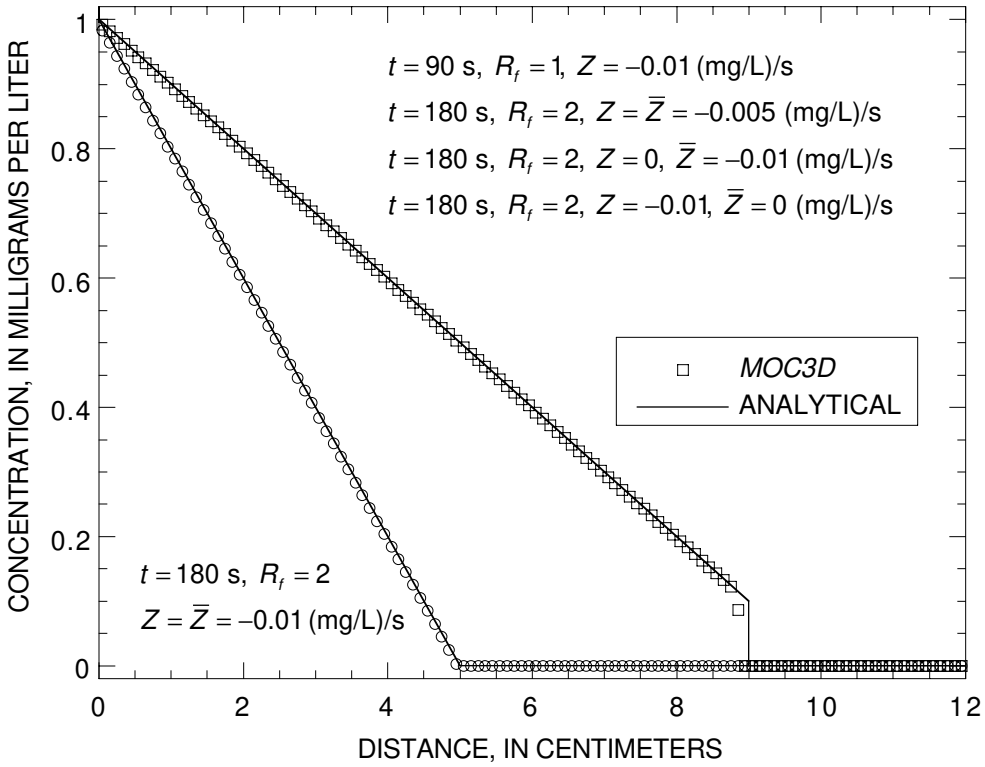

Figure 2. Numerical (*MOC3D*) and analytical solutions for several different cases for solute transport in a one-dimensional, steady flow field with zero-order loss and no dispersion. Variables are time, t, retardation factor, R_f, dissolved phase loss rate, Z, and sorbed phase loss rate, $\overline{Z}$. Other parameters are listed in table 5. [Abbreviations: s, second; mg/L, milligrams per liter]

Double-Porosity Exchange in One-Dimensional Steady Flow

The *MOC3D* extensions for double porosity *(DP)* are tested by comparing the numerical solution to an analytical solution for a one-dimensional steady-flow case. The physical system and model are generally the same as the one-dimensional case considered previously. The additional parameters for the immobile-water phase are listed in table 6. The initial concentration in the immobile phase is assumed to be zero and the initial concentration in the mobile phase is 20.0 in the first transport subgrid cell. This numerical initial condition approximates an instantaneous impulse condition at the inflow boundary. Incoming water has a concentration of zero, in contrast to

the case in the previous section. The linear velocity interpolation option is selected.

The governing equations are

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x} + \frac{\beta}{\varepsilon}\left(\tilde{C} - C\right) \quad \text{and} \quad (38)$$

$$\tilde{\varepsilon}\frac{d\tilde{C}}{dt} = \beta\left(C - \tilde{C}\right) \quad , \quad (39)$$

subject to the boundary conditions

$$0 = VC - D\frac{\partial C}{\partial x}, \qquad x = 0 \qquad (40)$$

$$\text{and} \qquad \frac{\partial C}{\partial x} = 0, \qquad x = L \qquad (41)$$

and the initial conditions:

$$C = 0\ , \quad \tilde{C} = 0, \quad 0 < x < L\ . \qquad (42)$$

The analytical solution for the solute concentration in the mobile phase for the case of an impulse inflow condition is given in the Laplace domain as (Valocchi, 1985)

$$\hat{C}(x,p) = \frac{2A\exp\left\{\frac{x}{2\alpha}\left[1-\left(1+4\frac{\alpha}{L}(fp+h)\right)\right]\right\}}{1+\left[1+4\frac{\alpha}{L}(fp+h)\right]^{1/2}}, \quad (43)$$

where $\hat{C}(x,p)$ is the Laplace transform of $C(x,t)$; p is the Laplace transform variable; $A = M/\varepsilon L^3$ where M is the total mass injected and L is a unit length (1 cm in the present case); α is the dispersivity and

$$h = \frac{(1-f)\omega p}{(1-f)p + \omega} \quad , \quad (44)$$

$$f = \frac{\varepsilon}{\varepsilon + \tilde{\varepsilon}} \quad , \text{ and} \quad (45)$$

$$\omega = \frac{\beta L}{\varepsilon v} \quad . \quad (46)$$

The concentration in the (x,t) domain is obtained by numerical inversion of the Laplace transform solution by use of the Stehfest algorithm (Stehfest, 1970; Moench and Ogata, 1984). The same numerical model parameters used in the decay test case (table 5) are used for this case, with the additional *DP* parameters listed in table 6.

Table 6. Modified and additional *MOC3D* parameters for double-porosity simulation. [s, seconds; mg/L, milligrams per liter]

Parameter	Value
Immobile-phase porosity ($\tilde{\varepsilon}$)	0.1
Exchange-rate coefficient (β)	varies
PERLEN (length of stress period)	60 s
Initial concentration (C_0)	
In first cell of transport subgrid (j=2)	20.0 mg/L
In other cells	0.0
Source concentration (C')	0.0
Initial concentration ($\tilde{C}$) in immobile-water phase	0.0
INTRPL (Interpolation scheme)	1

The analytical and *MOC3D* solutions agree well over a range of exchange-rate coefficient values (fig. 3). The numerical solution shows some minor deviations, especially at the peak concentrations for the case of $\beta = 0.001$ s^{-1}.

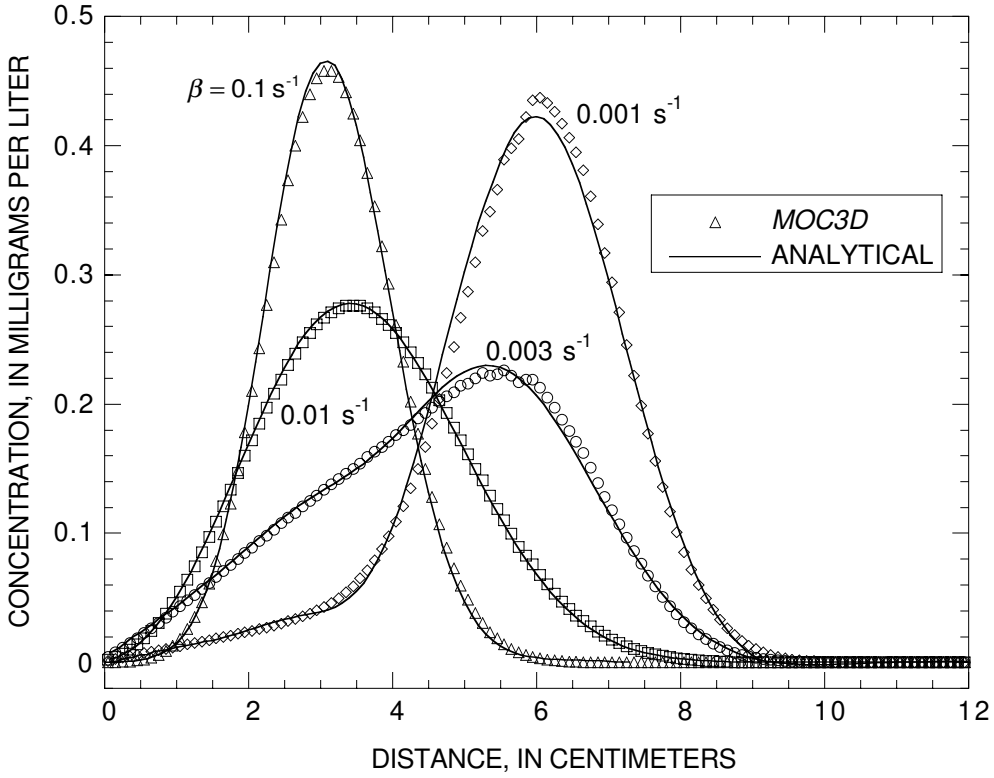

Figure 3. Numerical (*MOC3D*) and analytical solutions for several different cases for solute transport in a one-dimensional, steady flow field with double porosity. The variable is the linear exchange coefficient, β. Double-porosity parameters are listed in table 6 and other parameters are listed in table 5. [Abbreviation: s^{-1}, per second]

Age in One-Dimensional Steady Flow

The age transport solution is tested by comparing the numerical solution to an analytical solution for a one-dimensional steady-flow case with no dispersion. Under steady-flow conditions, the steady-state age distribution is obtained by solving a governing equation with the time derivative term set to zero. Thus, the governing equation and boundary condition for this case are

$$V\frac{dA}{dx} - \frac{\Sigma\left[W(0-A)\right]}{\varepsilon} - 1 = 0 \quad \text{, and} \tag{47}$$

$$0 = VA\ , \quad x = 0\ . \tag{48}$$

For the test problem here, the recharge term W is set to zero over the first half of the domain and takes on a non-zero uniform value over the second half as

$$\begin{aligned} W &= 0; \qquad 0 \le x \le L/2 \\ W &= \frac{\varepsilon}{A(x = L/2)}; \qquad L/2 < x \le L\ . \end{aligned} \tag{49}$$

By integration, the analytical solution where W=0 is

$$A = x/V \quad 0 \le x \le L/2 \quad . \tag{50}$$

For the properties used here, the age increases linearly from $A = 0$ at the inlet to the column to $A = 60$ s at $x = L/2 = 6$ cm.

To derive the solution for the last part of the column, the form of equation is changed from the flow-equation-removed form back to the form in which the divergence of water flux is included as

$$\frac{dqA}{dx} - WA' - \varepsilon = 0. \tag{51}$$

For W representing recharge with age zero, $WA' = 0$. By definition, $W = dq/dx$ for this one-dimensional problem. Splitting the derivative and substituting gives

$$q\frac{dA}{dx} + AW - \varepsilon = 0. \tag{52}$$

This expression can be integrated for the general case. A trivial solution is available for the case here by choosing $W = \varepsilon/A(x = L/2)$. In this case, the last two terms of (52) cancel, hence, $dA/dx = 0$. Thus, the analytical solution for the age is $A(6 \text{ cm} \le x \le 12 \text{ cm}) = 60$ s. The increase in age as water flows is precisely offset by the mixing of the water in the column with incoming water at age zero.

MOC3D cannot solve a steady-state transport equation directly, so the simulation is run for a time period long enough that the computed ages do not change appreciably with simulation time. Minor fluctuations or oscillations may continue to occur, but these are artifacts of the discrete numerical method. The input parameters for the model simulation are the same as those shown in table 5 except that the dispersivity is 0.0 and the simulation period length is 180 s.

The numerical solution agrees very well with the analytical solution (fig. 4). This case illustrates that the numerical methods used in *MOC3D* are suitable for advective transport problems in which dispersion is neglected. However, the model cannot solve steady-state transport problems directly but must be run in transient mode with constant conditions until steady-state conditions are asymptotically reached.

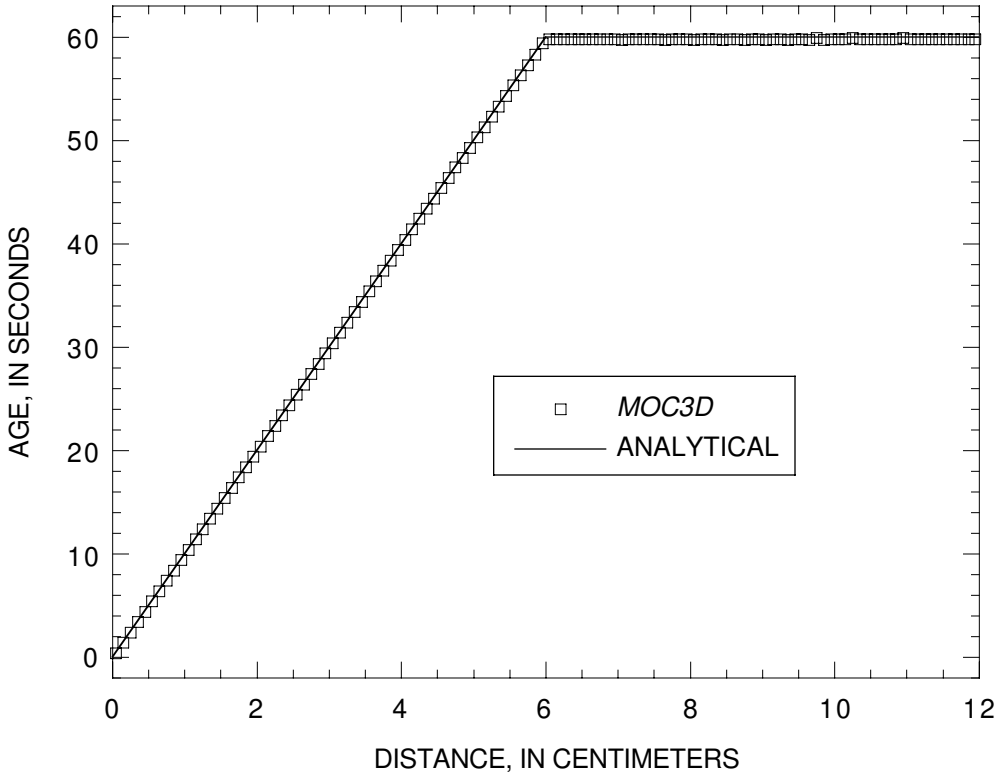

Figure 4. Numerical (*MOC3D*) and analytical solutions for ground-water age transport in a one-dimensional, steady flow field with no dispersion. Other parameters are listed in table 5.

SUMMARY AND CONCLUSIONS

The spatially variable and temporally variable geochemical conditions in contaminated aquifers lead to complex patterns of solute attenuation. These processes cannot be accurately approximated using uniform and constant reaction coefficients. To improve the capabilities of the ground-water solute transport model *MOC3D* to approximate these effects, simple reaction terms have been added to the governing equation and numerical methods, and the flexibility of existing reaction simulation has been improved. These modifications are incoporated in version 3.0 of *MOC3D*.

Recent advances in environmental tracers allows dating of ground water; the age of ground water is defined relative to isolation from the atmospheric source of the tracers. A useful tool in analysis of these age-dating results is a model of the age of ground water within an aquifer. *MOC3D* has been modified to simulate ground-water age transport, including the effects of double-porosity exchange.

The modifications described here extend the capabilities of *MOC3D* for simulation of solute transport in ground water. These extensions allow simulation of age transport, effects of diffusive exchange with an immobile-water phase, and more flexible retardation, decay, and growth reactions than those allowed in the original version of the model. These extensions are tested by comparing model output to analytical solutions

for special cases. These tests indicate that the model can generate accurate solutions to the ground-water transport equation for these special cases. These extensions do not alter the basic algorithms used to solve the transport equation, hence the guidance given by Konikow and others (1996) about applicability and accuracy of *MOC3D* for practical problems also applies to this version (3.0).

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APPENDIX A: ADDITIONAL DATA INPUT INSTRUCTIONS FOR AGE, DOUBLE POROSITY, AND SIMPLE REACTIONS IN *MOC3D (Version 3)*

All input variables are read using free formats, except as specifically indicated. In free format, variables are separated by one or more spaces or by a comma and optionally one or more spaces. Blank spaces are not read as zeros.

MOC3D Transport Name File (CONC)

FOR EACH SIMULATION:

1. Data: FTYPE NUNIT FNAME

The name file consists of records defining the names and units numbers of the files. Each "record" consists of a separate line of data. There must be a record for the listing file and for the main *MOC3D* input file.

The listing (or output) file ("CLST") must be the first record. The other files may be in any order. Each record can be no more than 79 characters.

FTYPE The file type, which may be one of the following character strings:

- ***CLST*** *MOC3D* listing file (separate from the *MODFLOW* listing file) *[required].*
- ***MOC*** or ***MOCIMP*** Main *MOC3D* input data file Specifying ***MOC*** indicates dispersion calculations will be explicit (as described by Konikow and others, 1996) and specifying ***MOCIMP*** indicates dispersion calculations will be implicit (as described by Kipp and others, 1998).
- ***CRCH*** Concentrations in recharge *[optional].*
- ***CNCA*** Separate output file containing concentration data in ASCII (text-only) format. Frequency and format controlled by NPNTCL and ICONFM *[optional].*
- ***CNCB*** Separate output file containing concentration data in binary format *[optional].*
- ***VELA*** Separate output file with velocity data in ASCII format. Frequency and format of printing controlled by NPNTVL and IVELFM *[optional].*
- ***VELB*** Separate output file with velocity data in binary format *[optional].*
- ***PRTA*** Separate output file with particle locations printed in ASCII format. Frequency and format of printing controlled by NPNTPL *[optional].*
- ***PRTB*** Separate output file with particle locations printed in binary format *[optional].*
- ***OBS*** Observation wells input file *[optional].*
- ***DATA*** For formatted files such as those required by the OBS package and for array data separate from the main *MOC3D* input data file *[optional].*
- ***DATA(BINARY)*** For unformatted input/output files *[optional].*

******* The following optional FTYPEs select modifications documented in this report ******

- ***AGE*** Ground-water age simulation input file *[optional].*
- ***DP*** Double porosity input file *[optional].*
- ***DK*** Simple reactions (decay, zero-order growth, retardation) input file *[optional].*

NUNIT The FORTRAN unit number used to read from and write to files. Any legal unit number other than 97, 98, and 99 (which are reserved by *MODFLOW*) can be used provided that it is not previously specified in the *MODFLOW* name file.

FNAME The name of the file.

AGE Input File

Activating the AGE package results in the model concentration output corresponding to ground-water ages. Age simulation is not compatible with most possible reaction terms in MOC3D, except for the double porosity option. Ground-water age is simulated with the advection dispersion transport equation by adding a uniform zero-order source term of unit (1) strength, corresponding to the rate of aging.

FOR EACH SIMULATION, IF *AGE* PACKAGE USED:

1. Data: AGER8 The aging rate (usually 1.0)

The aging rate (AGER8) is the ratio of model output age units to the simulation time units. If AGER8=1.0, the computed ages will be in the same time units as the transport simulation. AGER8 can be used to convert output ages to a more convenient time scale. For example, for output ages of years in a model simulation with time units of seconds, AGER8 = 1 / (365 * 24 * 60 * 60) = 1 / 31,536,000 = 3.171×10^{-8}.

Double Porosity (DP) Input File

Activating the double-porosity package allows simulation of linear kinetic exchange between the flowing water and an immobile water phase. Within the double-porosity package, options are provided to include decay and zero-order growth reactions. After a single line of control parameters, double-porosity properties are listed. Input includes the initial concentration, the porosity of the immobile phase, and the linear exchange coefficient. If optional reactions are selected, those rate coefficients also must be provided. The exchange-rate coefficient and the reaction-rate coefficients can optionally change each flow-model stress period.

FOR EACH SIMULATION, IF *DP* PACKAGE USED:

1. Data: IDPFO IDPZO IDPTIM IDPPS

IDPFO If IDPFO=1, activate first-order decay reaction in immobile water phase.

IDPZO If IDPZO=1, activate zero-order growth reaction in immobile water phase.

IDPTIM If IDPTIM=1, double porosity rate coefficients change each stress period.

IDPPS If IDPPS=1, print immobile-phase concentrations using aquifer-concentration formats and frequency.
If IDPPS=2, save immobile-phase concentrations using aquifer-concentration formats and frequency.
If IDPPS=3, print and save immobile-phase concentrations using aquifer-concentration formats and frequency.

FOR EACH LAYER OF TRANSPORT SUBGRID:

2. Data: DPCON(NSCOL,NSROW) Initial concentration [$\tilde{C}(t=0)$ (ML^{-3})].
Module: U2DREL*

3. Data: DPPOR(NSCOL,NSROW) Porosity of immobile water phase [$\tilde{\varepsilon}$ (-)].
Module: U2DREL*

FOR EACH SIMULATION (if IDPTIM=1, then FOR EACH FLOW-MODEL STRESS PERIOD)
FOR EACH LAYER OF TRANSPORT SUBGRID:

4. Data: DPXRAT(NSCOL,NSROW) Linear exchange coefficient [β (1/T)].
Module: U2DREL*

IF IDPFO=1, OPTIONAL FIRST-ORDER DECAY REACTION IN DOUBLE POROSITY

5. Data: DPFO(NSCOL,NSROW) First-order decay reaction coefficient [$\tilde{\lambda}$ (1/T)].
Module: U2DREL*

IF IDPZO=1, OPTIONAL ZERO-ORDER GROWTH REACTION IN DOUBLE POROSITY

6. Data: DPZO(NSCOL,NSROW) Zero-order growth reaction rate [$\tilde{Z}$ ($ML^{-3}T^{-1}$)].
Module: U2DREL*

For simulations using a multi-layer transport subgrid, input consists of 1, followed by 2 and 3 for each subgrid layer, followed by 4 and optionally 5 and 6 for each subgrid layer. If more than one flow-model stress period is used, and IDPTIM=1, then datasets 4 and optionally 5 and 6 are repeated for each subgrid layer, for each subsequent stress period.

Simple Reactions (DK) Input File

Activating the simple reactions package allows incorporation of simple but flexible reaction terms into the basic transport solution. The original model includes decay and retardation, but retardation is assumed to be uniform within each model layer. In the original model, decay is assumed to occur at the same rate in the dissolved and sorbed phases and is uniform throughout the model and constant during the entire simulation period. The DK package allows retardation factors to be input cell by cell. Decay also can be controlled cell by cell. In addition, decay can occur at different rates in the dissolved and sorbed phases, and the decay rates can change at the beginning of each flow model stress period. Finally, a zero-order growth reaction also is included; it also can be specified cell-by-cell and can optionally change at the beginning of each flow model stress period. After the initial control parameters, the retardation factors for all layers are read, if that option is activated (IDKRF=1). If read, these retardation factors overwrite the values read in the main MOC input file. Next, decay coefficients and growth rates are read layer by layer: all of the active decay and growth reaction terms for layer 1 are read, then the same parameters for layer 2, and so on. This grouping is used because when the time-variable reaction rates are used, and the retardation factor is not allowed to change in time. With the grouping used here, the decay and growth input structure for the initial stress period is the same as that used during subsequent stress periods.

FOR EACH SIMULATION, IF *DK* PACKAGE USED:

1. Data: IDKRF IDKTIM IDKFO IDKFS IDKZO IDKZS

IDKRF If IDKRF=1, activate spatially variable retardation factor.
IDKTIM If IDKTIM=1, decay and growth reaction rates change in time at each stress period.
IDKFO If IDKFO=1, activate spatially variable decay for dissolved phase.
IDKFS If IDKFS=1, activate spatially variable decay for sorbed phase.
IDKZO If IDKZO=1, activate spatially variable zero-order growth for dissolved phase.
IDKZS IF IDKZS=1, activate spatially variable zero-order growth for sorbed phase.

FOR EACH LAYER OF TRANSPORT SUBGRID:

IF IDKRF=1, OPTIONAL SPATIALLY VARIABLE RETARDATION FACTOR
2. Data: DKRF(NSCOL,NSROW) Retardation factor [R_f (-)].
Module: U2DREL*

FOR EACH SIMULATION (if IDKTIM=1, then FOR EACH FLOW-MODEL STRESS PERIOD)
FOR EACH LAYER OF TRANSPORT SUBGRID:

IF IDKFO=1, OPTIONAL DECAY RATE FOR DISSOLVED PHASE
3. Data: DKFO(NSCOL,NSROW) Decay rate coefficient for dissolved phase [λ (1/T)].
Module: U2DREL*

IF IDKFS=1, OPTIONAL DECAY RATE FOR SORBED PHASE
4. Data: DKFS(NSCOL,NSROW) Decay rate coefficient for sorbed phase [$\bar{\lambda}$ (1/T)].
Module: U2DREL*

IF IDKZO=1, OPTIONAL ZERO-ORDER GROWTH RATE IN DISSOLVED PHASE
5. Data: DKZO(NSCOL,NSROW) Zero-order growth rate for dissolved phase [Z ($ML^{-3}T^{-1}$)].
Module: U2DREL*

IF IDKZS=1, OPTIONAL ZERO-ORDER GROWTH RATE IN SORBED PHASE
6. Data: DKZS(NSCOL,NSROW) Zero-order growth reaction rate for sorbed phase [$\bar{Z}$ ($ML^{-3}T^{-1}$)].
Module: U2DREL*

Repeat 3-6, as needed, for each layer of the subgrid.

IF IDKTIM=1, Repeat 3-6, as needed, for all layers, for each flow-model stress period. Note that the retardation factor is constant in time and new values are not read for subsequent stress periods.

APPENDIX B: ANNOTATED EXAMPLE INPUT DATASET FOR SAMPLE PROBLEM

This example input dataset is for one of the solutions shown in figure 1 with retardation and decay in both sorbed and dissolved phases. Parameter values are listed in table 5. Several of the required data files (*finite.nam*, *finite.bas*, *finite.bcf*, and *finite.sip*) are those required for *MODFLOW-96*, and their formats are described by Harbaugh and McDonald (1996). Only files that are changed from the original documentation (Konikow and others, 1996) are reproduced here.

In the data files shown below, the right side of some data lines includes a semi-colon followed by text that describes the parameters for which values are given. These comments (including the semicolon) are not read by the program because in free format the code will only read the proper number of variables and ignore any subsequent information on that line. This style of commenting data files is optional, but users may find it helpful when viewing the content of data files.

Following (enclosed in a border) are the contents of the *MODFLOW* name file for the sample problem; explanations are noted outside of border:

File name: *finite.nam*

```
list     16      finite.lst   ← Designates main output file for MODFLOW
bas      95      finite.bas   ← Basic input data for MODFLOW
bcf      11      finite.bcf   ← Block-centered flow package
sip      19      finite.sip   ← Input for numerical solution of flow equation
conc     33      finite.mcn   ← Transport name file (turns transport "on")
  ↑       ↑          ↑
  1       2          3
```

1 Ftype (that is, the type of file)

2 Unit number

3 File name (name chosen to reflect contents of file)

Following (enclosed in a border) are the contents of the basic package input data file for the *MODFLOW* simulation of the sample problem; explanations are noted outside of border:

File name: *finite.bas*

```
Finite:  Compare to Wexler program and MOC3D                    BAS Input
      NLAY      NROW      NCOL      NPER     ITMUNI
         1         1       122         1          1
FREE
         0         1      ; IAPART,ISTRT
        95         1(25I3)                                    3   ; IBOUND
 -1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 -2
      0.00                                                ; HNOFLO
        95       1.0(122F5.0)                          1   ; HEAD
 12.1
 180.0           1        1.    ; PERLEN,NSTP,TSMULT
```

← 1
← 1
← 2
← 3
← 4
← 5
← 5
← 5
← 5
← 5
← 5
← 6
← 7
← 7
← 8

1 Two header lines of comments. For convenience and clarity, the second line is used to label names of parameters on subsequent line of file.

2 Flow grid dimensions, number of periods, and time units.

3 Options line (new in *MODFLOW-96*)

4 Flags for buffer array and drawdown calculations.

5 *IBOUND* identifiers (first line) and array

6 Head value assigned to inactive cells

7 Initial head information

8 *MODFLOW* time-step information

Following (enclosed in a border) are the contents of the *MOC3D* name file for the sample problem; explanations are noted outside of border:

File name: *finite.mcn*

```
clst      94       finite.out
moc       96       finite.moc
obs       44       finite.obs
data      45       finite.oba
cnca      22       finite.cna
cncb      23       finite.cnb
dk        24       finite.dk
```

← Designates main output file for *MOC3D*
← Main input data file for *MOC3D*
← Input data file for observation wells
← Output file for observation well data
← Separate output file for conc. data (ASCII)
← Separate output file for conc. data (binary)
← DK input data file (turns DK package "on")

↑ 1 ↑ 2 ↑ 3

1 Ftype

2 Unit number

3 File name

Following (enclosed in a border) are the contents of the main input data file for the *MOC3D* simulation for the sample problem; selected explanations are noted outside of border:

File name: *finite.moc*

```
One-dimensional, Steady Flow, DK Decay, Low Dispersion:  MOC3D 3.0 Input          ← 1
    ISLAY1    ISLAY2    ISROW1    ISROW2    ISCOL1    ISCOL2                     ← 1
         1         1         1         1         2       121                     ← 2
         0       0.0       0.0 ; NODISP, DECAY, DIFFUS                         ← 3
      2000         3           ; NPMAX, NPTPND                                  ← 4
       0.5      0.05         1 ; CELDIS, FZERO, INTRPL                          ← 4
  0 0 0 -1 0 0 0 ; NPNTCL, ICONFM, NPNTVL, IVELFM, NPNTDL, IDSPFM, NPRTPL       ← 5
       0.0       ; CNOFLO                                                       ← 6
         0       0.0 (122F3.0)                    ; initial concentration
         0       1.                               ; C' inflow
         2                                        ; NZONES to follow           ← 7
        -1       1.0                              ; IZONE, ZONCON              ← 7
        -2       0.0                              ; IZONE, ZONCON              ← 7
         0         0                              ; IGENPT                     ← 8
         0       0.1                              ; longitudinal disp.
         0       0.1                              ; transverse disp. horiz.
         0       0.1                              ; transverse disp. vert.
         0       1.0                              ; retardation factor
         0       1.0                              ; thickness
         0       0.1                              ; porosity
```

1 Two header lines of comments. For convenience and clarity, the second line is used to label names of parameters on subsequent line of file.

2 Indices for transport subgrid

3 Flag for no dispersion, decay rate, diffusion coefficient

4 Particle information for advective transport

5 Print flags

6 Value of concentration associated with inactive cells

7 Concentrations associated with fixed-head nodes (fixed head nodes are defined in the IBOUND array in the *MODFLOW* BAS package)

8 Flag for "strong" sources or sinks

Following (enclosed in a border) are the contents of the *DK* input data file for the *MOC3D* simulation for the sample problem; selected explanations are noted outside of border:

File name: *finite.dk*

```
   1   0   1   1   0   0 ; idkrf idktim idkfo idkfs idkzo idkzs                ← 1
CONSTANT  2.0                                                                  ← 2
CONSTANT  0.01                                                                 ← 3
CONSTANT  0.01                                                                 ← 4
```

1 Options for DK package

2 Spatially-variable retardation factors

3 Spatially-variable decay coefficient for dissolved phase

4 Spatially-variable decay coefficient for sorbed phase

APPENDIX C: SELECTED OUTPUT FOR SAMPLE PROBLEM

This example output was generated from the input datasets listed in appendix B for a case of one-dimensional transport in steady-state flow with retardation and decay. The line spacing and font sizes of the output files have been modified in places to enhance the clarity of reproduction in this report. Some repetitive lines of output have been deleted where indicated by an ellipsis (**...**).

Some brief annotations were added in a few places in this sample output listing to help the reader understand the purpose of various sections of output. These annotations are written in bold italics to clarify that they are not part of the output file.

Following are the contents of the *MOC3D* main output file for the sample problem.

```
             U.S. GEOLOGICAL SURVEY
METHOD-OF-CHARACTERISTICS SOLUTE TRANSPORT MODEL
          MOC3D (Version 3.0) 1999/03/24

MOC BASIC INPUT READ FROM UNIT
LISTING FILE: finite.out   UNIT  94

OPENING finite.moc
FILE TYPE: MOC   UNIT  96

OPENING finite.obs
FILE TYPE: OBS   UNIT  44

OPENING finite.oba
FILE TYPE: DATA   UNIT  45

OPENING finite.cna
FILE TYPE: CNCA   UNIT  22

OPENING finite.cnb
FILE TYPE: CNCB   UNIT  23

OPENING finite.dk
FILE TYPE: DK   UNIT  24
```

FILE INFORMATION

DK INPUT FILE

```
MOC BASIC INPUT READ FROM UNIT  96
```

2 TITLE LINES:

```
One-dimensional, Steady Flow, DK Decay, Low Dispersion:  MOC3D 3.0 Input
    ISLAY1    ISLAY2    ISROW1    ISROW2    ISCOL1    ISCOL2
```

PROBLEM DESCRIPTORS, INCLUDING GRID CHARACTERISTICS AND PARTICLE INFORMATION:

```
     MAPPING OF SOLUTE TRANSPORT SUBGRID IN FLOW GRID:
FIRST LAYER FOR SOLUTE TRANSPORT =   1      LAST LAYER FOR SOLUTE TRANSPORT  =   1
FIRST ROW FOR SOLUTE TRANSPORT   =   1      LAST ROW FOR SOLUTE TRANSPORT    =   1
FIRST COLUMN FOR SOLUTE TRANSPORT=   2      LAST COLUMN FOR SOLUTE TRANSPORT = 121

UNIFORM DELCOL AND DELROW IN SUBGRID FOR SOLUTE TRANSPORT

NO. OF LAYERS =    1   NO. OF ROWS =    1   NO. OF COLUMNS =  120
NO SOLUTE DECAY
NO MOLECULAR DIFFUSION
MAXIMUM NUMBER OF PARTICLES (NPMAX) =     2000
```

```
INPUT FOR DK OPTIONS READ FROM UNIT        24
 SPATIALLY-VARIABLE RETARDATION FACTOR
  LAYER-CONSTANT RETARDATION FACTORS FROM MOC INPUT FILE WILL NOT BE USED
 DECAY AND GROWTH RATES DO NOT CHANGE IN TIME
 SPATIALLY-VARIABLE FIRST-ORDER DECAY
 DISTINCT SPATIALLY-VARIABLE FIRST-ORDER DECAY FOR SORBED SOLUTE
  SORBED MASS DECAYS AT DIFFERENT RATE THAN DISSOLVED
 NO SPATIALLY-VARIABLE ZERO-ORDER GROWTH
 NO DISTINCT SPATIALLY-VARIABLE ZERO-ORDER GROWTH FOR SORBED SOLUTE
  SORBED MASS GROWS AT SAME RATE AS DISSOLVED

     240 ELEMENTS IN X ARRAY ARE USED BY DK
   14485 ELEMENTS IN X ARRAY ARE USED BY MOC
      12 ELEMENTS IN X ARRAY ARE USED BY OBS

 NUMBER OF PARTICLES INITIALLY IN EACH ACTIVE CELL (NPTPND) =   3
 PARTICLE MAP ("o" indicates particle location; shown as
             fractions of cell distances relative to node location):

      o------o------o

    -1/3     0     1/3

 INITIAL RELATIVE PARTICLE COORDINATES
   1    0.00000   0.00000  -0.33333
   2    0.00000   0.00000   0.00000
   3    0.00000   0.00000   0.33333

 CELDIS=     0.500
 FZERO =     0.050
```

D K OPTIONS

```
INTRPL= 1;  LINEAR INTERPOLATION SCHEME

NPNTCL=  0:     CONCENTRATIONS WILL BE WRITTEN AT THE END OF THE SIMULATION
MODFLOW FORMAT SPECIFIER FOR CONCENTRATION DATA: ICONFM=  0

NPNTVL=  0:         VELOCITIES WILL BE WRITTEN AT THE END OF THE SIMULATION
MODFLOW FORMAT SPECIFIER FOR      VELOCITY DATA: IVELFM= -1

NPNTDL=  0: DISP. COEFFICIENTS WILL NOT BE WRITTEN

NPNTPL=  0: PARTICLE LOCATIONS WILL NOT BE WRITTEN
```

OUTPUT CONTROL

```
CONCENTRATION WILL BE SET TO 0.00000E+00 AT ALL NO-FLOW NODES (IBOUND=0).

    INITIAL CONCENTRATION =  0.0000000E+00 FOR LAYER   1


VALUES OF C' REQUIRED FOR SUBGRID BOUNDARY ARRAY =    1
ONE FOR EACH LAYER IN TRANSPORT SUBGRID

ORDER OF C' VALUES: FIRST LAYER IN SUBGRID, EACH SUBSEQUENT LAYER,
LAYER ABOVE SUBGRID, LAYER BELOW SUBGRID:

  SUBGRID BOUNDARY ARRAY  =   1.000000


NUMBER OF ZONES FOR CONCENTRATIONS AT FIXED HEAD CELLS =    2

 ZONE FLAG =   -1     INFLOW CONCENTRATION =   1.0000E+00
 ZONE FLAG =   -2     INFLOW CONCENTRATION =   0.0000E+00

         SINK-SOURCE FLAG =              0 FOR LAYER   1
```

INITIAL AND BOUNDARY CONDITIONS FOR SOLUTE

```
 LONGITUDNL. DISPERSIVITY =  0.1000000

  HORIZ. TRANSVERSE DISP. =  0.1000000

   VERT. TRANSVERSE DISP. =  0.1000000

        RETARDATION FACTOR =   1.000000

         INITIAL THICKNESS =   1.000000     FOR LAYER   1

          INITIAL POROSITY =  0.1000000     FOR LAYER   1

  SIMPLE REACTION (DK) PACKAGE INPUT

   SPACE VAR. RETARD FCTR =   2.000000     FOR LAYER   1

  FIRST-ORDER DECAY COEF. =  0.1000000E-01 FOR LAYER   1

 FIRST-ORDER SORBED DECAY =  0.1000000E-01 FOR LAYER   1
```

DK INPUT

```
COORDINATES FOR   3 OBSERVATION WELLS:

  WELL #   LAYER     ROW  COLUMN    UNIT
       1       1       1       2      45
       2       1       1      42      45
       3       1       1     112      45
ALL OBSERVATION WELL DATA WILL BE WRITTEN ON UNIT  45

CONCENTRATION DATA WILL BE SAVED ON UNIT  22 IN ASCII FORMAT
CONCENTRATION DATA WILL BE SAVED ON UNIT  23 IN BINARY FORMAT

 TOTAL NUMBER OF PARTICLES GENERATED  =       360
 TOTAL NUMBER OF ACTIVE NODES (NACTIV) =       120
 MAX. NUMBER OF CELLS THAT CAN BE VOID OF PARTICLES (NZCRIT) =      6
     (IF NZCRIT EXCEEDED, PARTICLES ARE REGENERATED)
```

CALCULATED VELOCITIES (INCLUDING EFFECTS OF RETARDATION, IF PRESENT):

```
EFFECTIVE MEAN SOLUTE VELOCITIES IN COLUMN DIRECTION
                         AT NODES

1
  VELOCITY (COL)   IN LAYER  1 AT END OF TIME STEP  1 IN STRESS PERIOD  1
  ------------------------------------------------------------------------

          1        2        3        4        5        6        7        8        9     ...
 ..........................................................................................
   1  5.000E-02 5.000E-02 5.000E-02 5.000E-02 5.000E-02 5.000E-02 5.000E-02 5.000E-02 5.000E-02 ...

...
        111      112      113      114      115      116      117      118      119      120
 ..........................................................................................
   1  5.000E-02 5.000E-02 5.000E-02 5.000E-02 5.000E-02 5.000E-02 5.000E-02 5.000E-02 5.000E-02 5.000E-02

EFFECTIVE MEAN SOLUTE VELOCITIES IN ROW DIRECTION
                         AT NODES

1
  VELOCITY (ROW)   IN LAYER  1 AT END OF TIME STEP  1 IN STRESS PERIOD  1
  ------------------------------------------------------------------------

          1        2        3        4        5        6        7        8        9     ...
 ..........................................................................................
   1  0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 ...
```

```
...
       111       112       113       114       115       116       117       118       119       120
 ..........................................................................................................
   1   0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00

EFFECTIVE MEAN SOLUTE VELOCITIES IN LAYER DIRECTION
                         AT NODES
1
  VELOCITY (LAYER) IN LAYER  1 AT END OF TIME STEP  1 IN STRESS PERIOD  1
  ------------------------------------------------------------------------

         1         2         3         4         5         6         7         8         9     ...
 ..........................................................................................................
   1   0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 ...

...
       111       112       113       114       115       116       117       118       119       120
 ..........................................................................................................
   1   0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00


          STABILITY CRITERIA --- M.O.C.

     MAXIMUM FLUID VELOCITIES:  C-VEL =  5.00E-02     R-VEL =  1.00E-20     L-VEL =  1.00E-18
 MINIMUM TIME TO TRAVEL THCK =  1.00E+18

 TIMV =  1.00E+00     NTIMV  =    181

     MAX. C-VEL. IS CONSTRAINT AND OCCURS BETWEEN NODES (   2,   1,   1) AND (   1,   1,   1)

 TIMD =  1.00E+00     NTIMD  =    181

   THERE ARE NO FLUID SOURCES IN THE TRANSPORT SUBGRID

 NUMBER OF MOVES FOR ALL STABILITY CRITERIA:
    CELDIS  DISPERSION   INJECTION
       181         181           1

 CELDIS IS LIMITING
 DISPERSION IS LIMITING

          TIME STEP    1 IN STRESS PERIOD    1

          NO. OF PARTICLE MOVES REQUIRED TO COMPLETE THIS TIME STEP  =  181
            MOVE TIME STEP (TIMV)=  9.944751262665E-01
```

(NUMERICAL SOLUTION TO TRANSPORT EQUATION STARTS AT THIS POINT)

```
  NP      =     360 AT START OF MOVE        IMOV     =          1
  NP      =     360 AT START OF MOVE        IMOV     =          2
  NP      =     360 AT START OF MOVE        IMOV     =          3
  NP      =     360 AT START OF MOVE        IMOV     =          4
  NP      =     360 AT START OF MOVE        IMOV     =          5
...
  NP      =     360 AT START OF MOVE        IMOV     =        176
  NP      =     360 AT START OF MOVE        IMOV     =        177
  NP      =     360 AT START OF MOVE        IMOV     =        178
  NP      =     360 AT START OF MOVE        IMOV     =        179
```

ONE LINE PRINTED FOR EACH MOVE TO TRACK PROGRESS AND NUMBER OF ACTIVE PARTICLES

```
NP      =     360 AT START OF MOVE        IMOV     =        180
NP      =     360 AT START OF MOVE        IMOV     =        181

         SOLUTE BUDGET AND MASS BALANCE FOR TRANSPORT SUBGRID

    VALUES CALCULATED AT END OF:
             STRESS PERIOD    1  OUT OF    1
            FLOW TIME STEP    1  OUT OF    1
  TRANSPORT TIME INCREMENT  181  OUT OF  181

    ELAPSED TIME =  1.8000E+02

    CHEMICAL MASS IN STORAGE:
        INITIAL:   MASS DISSOLVED =  0.0000E+00     MASS SORBED =  0.0000E+00
        PRESENT:   MASS DISSOLVED =  4.1720E-02     MASS SORBED =  4.1720E-02

              CHANGE IN MASS STORED = -8.3440E-02

   CUMULATIVE SOLUTE MASS  (L**3)(M/VOL)
   ----------------------

        IN:
        ---
                   DECAY =  0.0000E+00
              CONSTANT HEAD =  0.0000E+00
        SUBGRID BOUNDARY =  1.8000E-01
                RECHARGE =  0.0000E+00
                   WELLS =  0.0000E+00
                  RIVERS =  0.0000E+00
                  DRAINS =  0.0000E+00
    GENL. HEAD-DEP. BDYS. =  0.0000E+00
       EVAPOTRANSPIRATION =  0.0000E+00
        FIRST-ORDER DECAY =  0.0000E+00
     1-ORDER DECAY SORBED =  0.0000E+00

                 TOTAL IN =  1.8000E-01

        OUT:
        ----
                   DECAY =  0.0000E+00
              CONSTANT HEAD =  0.0000E+00
         SUBGRID BOUNDARY = -1.8359E-05
                RECHARGE =  0.0000E+00
                   WELLS =  0.0000E+00
                  RIVERS =  0.0000E+00
                  DRAINS =  0.0000E+00
    GENL. HEAD-DEP. BDYS. =  0.0000E+00
       EVAPOTRANSPIRATION =  0.0000E+00
        FIRST-ORDER DECAY = -4.7825E-02
     1-ORDER DECAY SORBED = -4.7825E-02

                TOTAL OUT = -9.5668E-02


       SOURCE-TERM DECAY =  0.0000E+00



                RESIDUAL = -8.9162E-04

     PERCENT DISCREPANCY =  4.9534E-01 RELATIVE TO MASS FLUX IN
```

ITEMIZED BUDGETS FOR SOLUTE FLUXES

DK BUDGET