# MT3D

A Modular Three-Dimensional Transport Model
for Simulation of Advection, Dispersion and Chemical Reaction
of Contaminants in Groundwater Systems

By C. Zheng
S.S. Papadopulos & Associates, Inc
Rockville, Maryland  20852

Prepared for
The United States Environmental Protection Agency
Robert S. Kerr Environmental Research Laboratory
Ada, Oklahoma 74820

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# ABSTRACT

*mt3d: a modular three-dimensional transport model*

This documentation describes the theory and application of a modular three dimensional transport model for simulation of advection, dispersion and chemical reactions of dissolved constituents in groundwater systems. The model program, referred to as MT3D, uses modular structure similar to that implemented in MODFLOW, the U. S. Geological Survey (1988). This modular three-dimensional finite-difference groundwater flow model (McDonald and Harbaugh 1988). This modular structure makes it possible to simulate advection, dispersion, sink/source mixing, and chemical reactions independently without reserving computer memory space unused options. New transport processes and options can be added to the model readily without having to modify the existing code.

The MT3D transport model uses a mixed Eulerian-Lagrangian approach to the solution of the three-dimensional advective-dispersive-reactive equation, in three basic options: the method of characteristics (referred to as MOC), the modified method of characteristics (referred to as MMOC), and a hybrid of these two methods (referred to as HMOC). This approach combines the strength of the method of characteristics for eliminating numerical dispersion and the computational efficiency of the modified method of characteristics. The availability of both MOC and MMOC options, and their selective use based on an automatic adaptive procedure under the HMOC option, make MT3D uniquely suitable for a wide range of field problems.

T'he MT3D transport model is intended to be used in conjunction with any block-centered finite-difference flow model such as MODFLOW and is based on the assumption that changes in the concentration field wifl not affect the flow field measurably. This allows the user to construct and calibrate a flow model independently. MT3D retrieves the hydraulic heads and the various flow and sink/source terms saved by the flow model, automatically incorporating the specified hydrologic boundary conditions. Currently, MT3D accommodates the following spatial discretization capabilities and transport boundary conditions: (1) confined, unconfined variably confined/unconfined aquifer layers; (2) inclined model layers and variable cell thickness within the same layer, (3) specified concentration or mass flux boundaries; and (4) the solute transport effects of extemal sources and sinks such as wells, drains, rivers, areal recharge evapotranspiration.

# Chapter 1
# INTRODUCTION

## 1.1 PURPOSE AND SCOPE

Numerical modeling of contaminant transport, especially in three dimensions, is considerably more difficult than simulation of groundwater flow. Transport modeling not only is more vulnerable to numerical errors such as numerical dispersion and artificial oscillation, but also requires much more computer memory and execution time, making it impractical for many field applications, particularly in the micro-computer environment. There is obviously a need for a computer model that is virtually free of numerical dispersion and oscillation, simple to use and flexible for a variety of field conditions, and also efficient with respect to computer memory and execution time so that it can be run on most personal computers.

The new transport model documented in this report, referred to as MT3D, is a model for simulation of advection, dispersion and chemical reactions of contaminants in groundwater flow systems in either two or three dimensions. The model uses a mixed Eulerian-Lagrangian approach to the solution of the advective-dispersive-reactive equation, based on combination of the method of characteristics and the modified method of characteristics. This approach combines the strength of the method of characteristics for eliminating numerical dispersion and the computational efficiency of the modified method of characteristics. The model program uses a modular structure similar to that implemented in the U.S. Geologic Survey modular three-dimensional finite-difference groundwater flow model, referred to as MODFLOW, (McDonald and Harbaugh, 1988). The modular structure of the transport mode makes it possible to simulate advection, dispersion, source/sink mixing, or chemical reactions independently without reserving computer memory space for unused options; new packages involving other transport processes can be added to the model readily without having to the existing code.

The MT3D transport model was developed for use with any block-centered finite-difference flow model such as MODFLOW and is based on the assumption that changes in concentration field will not affect the flow field significantly. After a flow model is developed and calibrated, the information needed by the transport model can be saved in disk files which are then retrieved by the transport model. Since most potential users of a transport model are likely to have been familiar with one or more flow models, MT3D provides an opportunity to simulate contaminant transport without having to learn a new flow model or to modify an existing flow model to fit the transport model. In addition, separate flow simulation and calibration outside the transport model result in substantial savings in computer memory. The model structure also saves execution time when many transport runs are required while the flow solution remains the same. Although this report describes only the use of MT3D in conjunction with MODFLOW, MT3D can be linked to any other block-centered finite-difference flow model in a simple and straightforward fashion.

The MT3D transport model can be used to simulate changes in concentration of single--species miscible contaminants in groundwater considering advection, dispersion and some simple chemical reactions, with various types of boundary conditions and external sources or sinks. The chemical reactions included in the model are equilibrium-controlled linear or non-linear sorption and first-order irreversible decay or biodegradation. More, sophisticated chemical reactions can be added to the model without changing the existing code. Currently, MT3D accommodates the following spatial discretization capabilities and transport boundary conditions: (1) confined, unconfined or variably confined/unconfined aquifer layers; (2) inclined model layers and variable cell thickness within the same layer; (3) specified concentration or mass flux boundaries; and (4) the solute transport effects of external sources and sinks such as wells, drains, rivers, areal recharge and evapotranspiration.

## 1.2 SOLUTION TECHNIQUES

The advective-dispersive-reactive equation describes the transport of miscible contaminants in groundwater flow systems. Most numerical methods for solving the advective-dispersive-reactive equation can be classified as Eulerian, Lagrangian or mixed Eulerian-Lagrangian (Neuman 1984). In the Eulerian approach, the transport equation is solved with a fixed grid method such as the finite-difference or finite-element method. The Eulerian approach offers the advantage and convenience of a fixed grid, and handles dispersion/reaction dominated problems effectively. For advection-dominated problems which exist in many field conditions, however, an Eulerian method is susceptible to excessive numerical dispersion or oscillation, and limited by small grid spacing and time steps. In the Lagrangian approach, the transport equation is solved in either a deforming grid or deforming coordinate in a fixed grid. The Lagrangian approach provides an accurate and efficient solution to advection dominated problems with sharp concentration fronts. However, without a fixed grid or coordinate, a Lagrangian method can lead to numerical instability and computational difficulties in nonuniform media with multiple sinks/sources and complex boundary conditions (Yeh, 1990). The mixed Eulerian-Lagrangian approach attempts to combine the advantages of both the Eulerian and the Lagrangian approaches by solving the advection term with a Lagrangian method and the dispersion and reaction terms with an Eulerian method.

The numerical solution implemented in MT3D is a mixed Eulerian-Lagrangian method. The Lagrangian part of the method, used for solving the advection term, employs the forward tracking method of characteristics (MOC), the backward-tracking modified method of characteristics (MMOC), or a hybrid of these two methods. The Eulerian part of the method, used for solving the dispersion and chemical reaction terms, utilizes a conventional block-centered finite-difference method.

The method of characteristics, which was implemented in the U.S. Geological Survey two-dimensional solute transport model (Konikow and Bredehoeft, 1978), has been use extensively in field studies. The MOC technique solves the advection term with a set of moving particles, and virtually eliminates numerical dispersion for sharp front problems. One major drawback of this technique is that it needs to track a large number of moving particles, especially for three-dimensional simulations, consuming a large amount of both computer memory and execution time. The modified method of characteristics (MMOC) (e.g., Wheeler and Russell, 1983; Cheng et. al., 1984) approximates the advection term by directly tracking the nodal points of a fixed grid backward in time, and by using interpolation techniques. The MMOC technique eliminates the need to track and maintain a large number of moving particles; therefore, it requires much less computer memory and generally is more efficient computationally than the MOC technique. The disadvantage of the MMOC technique is that it introduces some numerical dispersion when sharp concentration fronts are present. The hybrid MOC/MMOC technique (e.g., Neuman, 1984; Farmer, 1987) attempts to combine the strengths of the MOC and the MMOC techniques based on automatic adaptation of the solution process to the nature of the concentration field. The automatic adaptive procedure implemented in MT3D is conceptually similar to the one proposed by Neuman (1984). When sharp concentration fronts are present, the advection term is solved by the forward-tracking MOC technique through the use of moving particles dynamically distributed around each front. Away from such fronts, the advection term is solved by the MMOC technique with nodal points directly tracked backward in time. When a front dissipates due to dispersion and chemical reactions, the forward tracking stops automatically and the corresponding particles are removed.

The MT3D transport model uses an explicit version of the block-centered finite-difference method to solve the dispersion and chemical reaction terms. The limitation of an explicit scheme is that there is a certain stability criterion associated with it, so that the size of time steps cannot exceed a certain value. However, the use of an explicit scheme is justified by the fact that it saves a large amount of computer memory which would be required by a matrix solver used in an implicit scheme. In addition, for many advection-dominated problems, the size of transport steps is dictated by the advection process, so that the stability criterion associated with the scheme for the dispersion and reaction processes is not a factor. It should be noted that a solution package based on implicit schemes for solving dispersion and reactions could easily be developed and added to the model as an alternative solver for mainframes, more powerful personal computers, or workstations with less restrictive memory constraints.

## 1.3 ORGANIZATION OF THIS REPORT

This report covers the theoretical, numerical and application aspects of the MT3D transport model. Following this introduction, Chapter 2 gives a brief overview of the mathematical-physical basis and various functional relationships underlying the transport model. Chapter 3 explains the mixed Eulerian-Lagrangian solution schemes used in MT3D in more detail. Chapter 4 discusses implementational issues of the numerical method. Chapter 5 describes the structure and design of the MT3D model program, which has been divided into main program and a number of packages, each of which deals with a single aspect of the transport simulation. Chapter 6 provides detailed model input instructions and discusses how to set up a simulation. Chapter 7 describes the example problems that were used to verify and test the MT3D program The appendices include information on the computer memory requuements of the MT3D model and its interface with a flow model; printout of sample input and files; explanation of several post-processing programs and tables of abbreviated input instructions.

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# Chapter 2
# FUNDAMENTALS OF THE TRANSPORT MODEL

## 2.1 GOVERNING EQUATIONS

The partial differential equation describing three-dimensional transport of contaminants in groundwater can be written as follows (e.g., Javandel, et. al., 1984):

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(v_i C) + \frac{q_s}{\theta}C_s + \sum_{k=1}^{N} R_k \qquad (2.1)$$

where

C is the concentration of contaminants dissolved in groundwater, $ML^{-3}$;

*t* is time, T;

$X_i$ is the distance along the respective Cartesian coordinate axis, L;

$D_{ij}$ is the hydrodynamic dispersion coefficient, $L^2T^{-1}$

$v_j$ is the seepage or linear pore water velocity, $LT^{-1}$;

$q_s$ is the volumetric flux of water per unit volume of aquifer representing sources (positive) and sinks (negative), $T^{-1}$ ;

$C_s$ is the concentration of the sources or sinks, $ML^{-3}$;

$\theta$ is the porosity of the porous medium dimensionless;

$\sum_{k=1}^{N} R_k$ is a chemical reaction term, $ML^{-3}T^{-1}$.

Assuming that only equilibrium-controlled linear or non-linear sorption and first-order irreversible rate reactions are involved in the chemical reactions, the chemical reaction term in equation (2.1) can be expressed as (Grove and Stollenwerk, 1984):

$$\sum_{k=1}^{N} R_k = \frac{\rho_b}{\theta}\frac{\partial \overline{C}}{\partial t} - \lambda\left(C + \frac{\rho_b}{\theta}\overline{C}\right) \qquad (2.2)$$

where

$P_b$ is the bulk density of the porous medium, $ML^{-3}$;

$\overline{C}$ is the concentration of contaminants sorbed on the porous medium, $MM^{-1}$;

8 is the rate constant of the first-order rate reactions, T-1

By rewriting the $\frac{\rho_b}{\theta}\frac{\partial \overline{C}}{\partial t}$ term as:

$$\frac{\rho_b}{\theta}\frac{\partial \overline{C}}{\partial t} = \frac{\rho_b}{\theta}\frac{\partial C}{\partial t}\frac{\partial \overline{C}}{\partial C} \tag{2.3}$$

and substituting equations (2.2) and (2.3) into equation (2.1), the following equation is obtained:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(v_i C) + \frac{q_s}{\theta}C_s + \frac{\rho_b}{\theta}\frac{\partial \overline{C}}{\partial C}\frac{\partial C}{\partial t} - \lambda\left(C + \frac{\rho_b}{\theta}\overline{C}\right) \tag{2.4}$$

Moving the fourth term on the right-hand side of equation (2.4) to the left-hand side, equation (2.4) becomes:

$$R\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(v_i C) + \frac{q_s}{\theta}C_s - \lambda\left(C + \frac{\rho_b}{\theta}\overline{C}\right) \tag{2.5}$$

where R is called the retardation factor, defined as

$$R = 1 + \frac{\rho_b}{\theta}\frac{\partial \overline{C}}{\partial C} \tag{2.6}$$

Equation (2.5) is the governing equation underlying in the transport model. The transport equation is linked to the flow equation through the relationship:

$$v_i = -\frac{K_{ii}}{\theta}\frac{\partial h}{\partial x_i} \tag{2.7}$$

where

$K_{ii}$ is a principal component of the hydraulic conductivity tensor, $LT^{-1}$

$h$ is hydraulic head, L.

The hydraulic head is obtained from the solution of the three-dimensional groundwater flow equation:

$$\frac{\partial}{\partial x_i}\left(K_{ii}\frac{\partial h}{\partial x_j}\right) + q_s = S_s\frac{\partial h}{\partial t} \tag{2.8}$$

where

S, is the specific storage of the porous materials, $L^{-1}$.

Note that the hydraulic conductivity tensor (K) actually has nine components. However, it is generally assumed that the principal components of the hydraulic conductivity tensor *($K_{ii}$, or $K_{xx}$, $K_{yy}$, $K_{zz}$.)* are aligned with the x, y and z coordinate axes so that non-principal components become zero. This assumption is incorporated in most commonly used flow models, including MODFLOW.

## 2.2 ADVECTION

The second term on the right-hand side of equation (2.5), $\frac{\partial}{\partial x_i}(v_i C)$ , is referred to as the advection term. The advection term describes the transport of miscible contaminants at the same velocity as the groundwater. For many practical problems concerning contaminant transport in groundwater, the advection term dominates. To measure the degree of advection domination, a dimensionless Peclet number is usually used. The Peclet number is defined as:

$$P_e = \frac{|v|L}{D} \tag{2.9}$$

where

$|v|$ is the magnitude of the seepage velocity vector, $LT^{-1}$;

$L$ is a characteristic length, commonly taken as the grid cell width, L;

$D$ is the dispersion coefficient, $L^2T^{-1}$.

In advection-dominated problems, also referred to as sharp front problems, the Peclet number has a large value. For pure advection problems, the Peclet number becomes infinite.

For advection-dominated problems, the solution of the transport equation by many standard numerical procedures is plagued to some degree by two types of numerical problems as illustrated in Fig. 2.1. The first type is numerical dispersion, which has an effect similar to that of physical dispersion, but is caused by truncation error. When physical dispersion is small or negligible, numerical dispersion becomes a serious problem, leading to the smearing of concentration fronts which should have a sharp appearance (Fig. 2. la). The second type of numerical problem is artificial oscillation, sometimes also referred to as overshoot and undershoot, as illustrated in Fig. 2.lb. Artificial oscillation is typical of many higher-order schemes designed to eliminate numerical dispersion, and tends to become more severe as the concentration front becomes sharper.

The mixed Eulerian-Lagrangian method implemented in the MT3D transport model is virtually free of numerical dispersion and artificial oscillation and is capable of handling the entire range of Peclet numbers from 0 to $\infty$ as discussed in the next chapter.

## 2.3 DISPERSION

### 2.3.1 Dispersion Mechanism

Dispersion in porous media refers to the spreading of contaminants over a greater regionthan would be predicted solely from the groundwater velocity vectors. As described by Anderson (1984), dispersion is caused by mechanical dispersion, a result of deviations of actual velocity on a microscale from the average groundwater velocity, and molecular diffusion, a result of concentration variations. The molecular diffusion effect is generally secondary and negligible compared to the mechanical dispersion effect, and only becomes important when groundwater velocity is very low. The sum of the mechanical dispersion and the molecular diffusion is termed hydrodynamic dispersion.

Fig. 2.1. Illustration of common numerical errors in contaminant transport modeling.

Although the dispersion mechanism is generally understood, the representation of dispersion phenomena in a transport model is the subject of intense continuing research. The dispersion term in equation (2.5), $\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right)$ represents a pragmatic approach through which realistic transport calculations can be made without fully describing the heterogeneous velocity field, which, of course, is impossible to do in practice. While many different approaches and theories have been developed to represent the dispersion process, equation (2.5) is still the basis for most practical simulations.

### 2.3.2 Dispersion Coefficient

The hydrodynamic dispersion tensor for isotropic porous media is defined, according to Bear (1979), in the following component forms:

$$D_{xx} = \alpha_L \frac{v_x^2}{|v|} + \alpha_T \frac{v_y^2}{|v|} + \alpha_T \frac{v_z^2}{|v|} + D^* \qquad (2.9a)$$

$$D_{yy} = \alpha_L \frac{v_y^2}{|v|} + \alpha_T \frac{v_x^2}{|v|} + \alpha_T \frac{v_z^2}{|v|} + D^* \tag{2.9b}$$

$$D_{zz} = \alpha_L \frac{v_z^2}{|v|} + \alpha_T \frac{v_x^2}{|v|} + \alpha_T \frac{v_y^2}{|v|} + D^* \tag{2.9c}$$

$$D_{xy} = D_{yx} = (\alpha_L - \alpha_T) \frac{v_x v_y}{|v|} \tag{2.9d}$$

$$D_{xz} = D_{zx} = (\alpha_L - \alpha_T) \frac{v_x v_z}{|v|} \tag{2.9e}$$

$$D_{yz} = D_{zy} = (\alpha_L - \alpha_T) \frac{v_y v_z}{|v|} \tag{2.9f}$$

where

"$_L$ is the longitudinal dispersivity, L;

"$_T$ is the transverse dispersivity, L;

$D*$ is the effective molecular diffusion coefficient, $L^2T^{-1}$ ;

$v_x$, $v_y$, $v_z$, are components of the velocity vector along the x, y, and z axes, $LT^{-1}$;

$|v| = (v_x^2 + v_y^2 + v_z^2)^{1/2}$ is the magnitude of the velocity vector, $LT^{-1}$.

Strictly speaking, the dispersion tensor defined by two independent dispersivities for isotropic media as in equations (2.9a) to (2.9f) is not valid for anisotropic porous media, which require five independent dispersivities (Bear, 1979). Unfortunately, it is generally not feasible to obtain all five dispersivities in the field. As a result, the usual practice in transport modeling is to assume that the isotropic dispersion coefficient is also applicable to anisotropic porous media.

In addition to the isotropic dispersion described above, the MT3D transport model supports an alternative form which allows the use of two transverse dispersivities, a horizontal transverse dispersivity ("$_{TH}$) and a vertical transverse dispersivity ("$_{TV}$), as proposed by Burnett and Frind (1987):

$$D_{xx} = \alpha_L \frac{v_x^2}{|v|} + \alpha_{TH} \frac{v_y^2}{|v|} + \alpha_{TV} \frac{v_z^2}{|v|} + D^* \tag{2.10a}$$

$$D_{yy} = \alpha_L \frac{v_y^2}{|v|} + \alpha_{TH} \frac{v_x^2}{|v|} + \alpha_{TV} \frac{v_z^2}{|v|} + D^* \tag{2.10b}$$

$$D_{zz} = \alpha_L \frac{v_z^2}{|v|} + \alpha_{TV} \frac{v_x^2}{|v|} + \alpha_{TV} \frac{v_y^2}{|v|} + D^* \tag{2.10c}$$

$$D_{xy} = D_{yx} = (\alpha_L - \alpha_{TH}) \frac{v_x v_y}{|v|} \tag{2.10d}$$

$$D_{xz} = D_{zx} = (\alpha_L - \alpha_{TH}) \frac{v_x v_z}{|v|} \tag{2.10e}$$

$$D_{yz} = D_{zy} = (\alpha_L - \alpha_{TH}) \frac{v_y v_z}{|v|} \tag{2. 10f}$$

Equations (2.10a) to (2.10f) become equivalent to equations (2.9a) to (2.9f) when the two transverse dispersivities are set equal.

## 2.4 SINKS AND SOURCES

The third term in the governing equation, $\frac{q_s}{\theta} C_s$ , is the sink/source term, which represents solute mass dissolved in water entering the simulated domain through sources, or solute mass dissolved in water leaving the simulated domain through sinks.

Sinks or sources may be classified as areally distributed or point sinks or sources. The areally distributed sinks or sources include recharge and evapotranspiration. The point sinks or sources include wells, drains, and rivers. Constant-head and general head dependent boundaries in the flow model are also treated as point sinks or sources because they function in exactly the same way as wells, drains, or rivers in the transport model.

For sources, it is necessary to specify the concentration of source water. For sinks, the concentration of sink water is generally equal to the concentration of groundwater in the aquffer and should not be specified. However, there is one exception where the concentration of sinks may differ from that of groundwater. The exception is evapotranspiration, which may be assumed to take only pure water away from the aquifer so that the concentration of the evapotranspiration flux is zero.

## 2.5 CHEMICAL REACTIONS

The chemical reactions included in the MT3D transport model are equilibrium-controlled linear or non-linear sorption and first-order irreversible rate reactions -- most commonly, radioactive decay or biodegradation. More sophisticated chemical reactions can be added to the model when necessary without modifying the existing program.

### 2.5.1 Linear or Non-linear Sorption

Sorption refers to the mass transfer process between the contaminants dissolved in groundwater (solution phase) and the contaminants sorbed on the porous medium (solid phase). It is generally assumed that equilibrium conditions exist between the solution-phase and solid--phase concentrations and that the sorption reaction is fast enough relative to groundwater velocity so that it can be treated as instantaneous. The functional relationship between the dissolved and sorbed concentrations is called the sorption isotherm. Sorption isotherms are generally incorporated into the transport model through the use of the retardation factor (e.g., Goode and Konikow, 1989). Three types of sorption isotherms are considered in the MT3D transport model: linear, Freundlich and Langmuir.

The linear sorption isotherm assumes that the sorbed concentration ( $\overline{C}$ ) is directly proportional to the dissolved concentration (C):

$$\overline{C} = K_d C \tag{2.11}$$

where ,$K_d$ is called the distribution coefficient, $L^3M^{-1}$. The retardation factor is defined as

$$R = 1 + \frac{\rho_b}{\theta}\frac{\partial \overline{C}}{\partial C} = 1 + \frac{\rho_b}{\theta} K_d \tag{2.12}$$

The Freundlich isotherm is a non-linear isotherm, expressed in the following form:

$$\overline{C} = K_f C^{a} \tag{2.13}$$

where

$K_f$ is the Freundlich constant, $(L^3M^{-1})^a$;

$a$ is the Freundlich exponent, dimensionless.

Both $K_f$ *and a* are empirical coefficients. When $a$ is equal to 1, the Freundlich isotherm is equivalent to the linear isotherm. The retardation factor for the Freundlich isotherm is defined accordingly as:

$$R = 1 + \frac{\rho_b}{\theta}\frac{\partial \overline{C}}{\partial C} = 1 + \frac{\rho_b}{\theta} a K_f C^{a-1} \tag{2.14}$$

Another non-linear sorption isotherm is the Langmuir isotherm, described by

$$\overline{C} = \frac{K_l \overline{S} C}{1 + K_l C} \tag{2.15}$$

where

$K_l$ is the Langmuir constant, $L^3M^{-1}$

$\overline{S}$ is the total concentration of sorption sites available, $MM^{-1}$.

The retardation factor defined for the Langrnuir isotherm is then

$$R = 1 + \frac{\rho_b}{\theta}\frac{\partial \overline{C}}{\partial C} = 1 + \frac{\rho_b}{\theta}\left[\frac{K_l \overline{S}}{(1 + K_l C)^2}\right] \tag{2.16}$$

### 2.5.2 Radioactive Decay or Biodegradation

The first-order irreversible rate reaction term included in the governing equation, $-\lambda\left(C + \frac{\rho_b}{\theta}\overline{C}\right)$ , represents the mass loss of both the dissolved phase (C) and the sorbed phase $(\overline{C})$ with the same rate constant rate (8). The rate constant is usually given in terms of the half-life:

$$\lambda = \frac{(\ln 2)}{t_{1/2}} \qquad (2.17)$$

where $t_{1/2}$ is the half-life of radioactive or biodegradable materials, or the time required for the concentration to decrease to one-half of the original value.

For certain types of biodegradation, the rate constant for the dissolved and sorbed phases may be different. Thus, in the MT3D model, two general rate constants are used: one for the dissolved phase ($8_1$) and the other for the sorbed phase ($8_2$) as shown below:

$$-\lambda\left(C + \frac{\rho_b}{\theta}\overline{C}\right) = -\lambda_1 C - \lambda_2\frac{\rho_b}{\theta}\overline{C} \qquad (2.18)$$

The two constants should be set equal if the rate reaction simulated is radioactive decay, since radioactive decay generally occurs at the same rate in both phases. If the simulated reaction is biodegradation, the two rate constants can be entered as different values.

It should be noted that the biodegradation process in the subsurface is complex and often does not follow the first-order rate reaction equation (e.g., Suflita, et. al., 1987). Alternative formulation for simulating biodegradation could be developed and added to the MT3D model as a new option in the future.

## 2.6 INITIAL CONDITIONS

The governing equation of the transport model describes the transient changes of solute concentration in groundwater. Therefore, initial conditions are necessary to obtain a solution of the governing equation. The initial condition in general form is written as

$$C(x,y,z,t) = C^{\circ}(x,y,z) \;\; on \;\; \forall, \qquad t \geq 0 \qquad (2.19)$$

where

*CE (x, y, z)* is a known concentration distribution and œ denotes the simulated domain.

## 2.7 BOUNDARY CONDITIONS

The solution of the governing equation also requires specification of boundary conditions. Three general types of boundary condition are considered in the MT3D transport model: (a) concentration known around a boundary (Dirichlet Condition), (b) concentration gradient known across a boundary (Neumann Condition); and (c) a combination of (a) and (b).

For the first type of boundary condition, the concentration is specified along the boundary and remains unchanged throughout the simulation, or,

$$C(x,y,z,t) = C^{\circ}(x,y,z) \;\; on \;\; \Gamma_1, \qquad t=0 \tag{2.20}$$

where '$_1$, denotes the specified-concentration boundary, and *CE(x,y,z)* is the specified concentration along '$_1$.

In a flow model, a Dirichlet boundary is a specified-head boundary which acts as a source or sink of water entering or leaving the simulated domain. Similarly, a specified-concentration boundary in a transport model acts as a source providing solute mass to the unulated domain, or as a sink taking solute mass out of the simulated domain. A specified-head boundary in the flow model may or may not be a specified-concentration boundary in the transport model.

For the second type of boundary condition, the concentration gradient is specified across the boundary, or,

$$D_{ij}\frac{\partial C}{\partial x_j} = q(x,y,z,t) \;\; on \;\; \Gamma_2, \qquad t \geq 0 \tag{2.21}$$

where *q(x, y, z, t)* is a known function representing the dispersive flux normal to the boundary '$_2$. A special case is along impermeable boundaries where *q(x, y, z, t)* = 0.

For the third type of boundary condition, both the concentration and concentration gradient are specified, or,

$$D_{ij}\frac{\partial C}{\partial x_j} - v_i C = g(x,y,z,t) \;\; on \;\; \Gamma_3, \; t \geq 0 \tag{2.22}$$

where *g(x, y, z, t)* is a known function representing the total flux (dispersive and advective) normal to the boundary '$_3$. For impermeable boundaries, both dispersive and advective fluxes are equal to zero so that *g(x, y, z, t) = 0*. On inflow or outflow boundaries, it is customary to assume that the advective flux dominates over the dispersive flux so that the above equation can be simplified to

$$-v_t C = g(x,y,z,t) \tag{2.23}$$

Equation (2.23) can be accommodated readily in the sink/source term of the governing equation.

# Chapter 3
# EULERIAN-LAGRANGIAN SOLUTION

## 3.1 EULERIAN-LAGRANGIAN EQUATIONS

According to the chain rule, the advection term in governing equation (2.5) can be expanded to

$$\frac{\partial}{\partial x_i}(v_i C) = v_i \frac{\partial C}{\partial x_i} + C \frac{\partial v_i}{\partial x_i} = v_i \frac{\partial C}{\partial x_i} + C \frac{q_s}{\theta} \tag{3.1}$$

Substituting equation (3. 1) into equation (2.5) and dividing both sides by the retardation factor, the governing equation becomes

$$\frac{\partial C}{\partial t} = \frac{1}{R} \frac{\partial}{\partial x_i}\left( D_{ij} \frac{\partial C}{\partial x_j} \right) - \overline{v}_i \frac{\partial C}{\partial x_i} - \frac{q_s}{R\theta}(C - C_s) - \frac{\lambda}{R}\left( C + \frac{\rho_b}{\theta} \overline{C} \right) \tag{3.2}$$

where, $\overline{v}_i = \frac{v_i}{R}$ , represents the "retarded" velocity of a contaminant particle.

Equation (3.2) is an Eulerian expression in which the partial derivative, $\left( \frac{\partial C}{\partial t} \right)$ , indicates the rate of change in solute concentration (C) at a fixed point in space. Equation (3.2) can also be expressed in the Lagrangian form as

$$\frac{DC}{Dt} = \frac{1}{R} \frac{\partial}{\partial x_i}\left( D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{q_s}{R\theta}(C - C_s) - \frac{\lambda}{R}\left( C + \frac{\rho_b}{\theta} \overline{C} \right) \tag{3.3}$$

where the substantial derivative, $\frac{DC}{Dt} = \frac{\partial C}{\partial t} + \overline{v}_i \frac{\partial C}{\partial x_i}$, indicates the rate of change in solute concentration (C) along the pathline of a contaminant particle (or a characteristic curve of the velocity field).

By introducing the finite-difference algorithm, the substantial derivative in equation (3.3) can be approximated as

$$\frac{DC}{Dt} = \frac{C_m^{n+1} - C_m^{n^*}}{\Delta t} \tag{3.4}$$

so that equation (3.3) becomes

$$C_m^{n+1} = C_m^{n^*} + \Delta t \times RHS \tag{3.5}$$

where

$C_m^{n+1}$ is the average solute concentration for cell m at the new time level *(n+1)*;

$C_m^{n^*}$ is the average solute concentration for cell *m* at the new time level *(n+l)* due to advection alone, also referred to as the intermediate time level *(n*);*

$\Delta t$ is the time increment between the old time level *(n)* and the new time level *(n+l);*

*RHS* represents the finite-difference approximation to the terms on the right-hand side of equation (3.3). The finite-difference approximation is explicit if the concentration at the old time level $C^n$ is used in the calculation of *RHS;* it is implicit if the concentration at the new time level $C^{n+1}$ is used.

Equation (3.5) constitutes the basic algorithm of the mixed Eulerian-Lagrangian method used in the MT3D transport model. In this method, the term $C_m^{n^*}$ in equation (3.5), which accounts for the effect of advection, is solved with a Lagrangian method on a moving coordinate, while the second term in equation (3.5), which accounts for the effects of dispersion, sink/source mixing, and chemical reactions, is solved with a finite-difference method on the fixed Eulerian grid.

Depending on the use of different Lagrangian techniques to approximate the advection term, the mixed Eulerian-Lagrangian method may be classified as: the method of characteristics (e.g., Garder et. al., 1964; Konikow and Bredehoeft, 1978); the modified method of characteristics (e.g., Russell and Wheeler, 1983; Cheng et. al., 1984); and a combination of the two (e.g., Neuman, 1984; Farmer, 1987). Each of these three solution schemes is utilized in the MT3D transport model. The concepts and the fundamental ideas behind these solution schemes are discussed briefly in the next three sections. The numerical implementation of these solution schemes is presented in detail in Chapter 4.

## 3.2 METHOD OF CHARACTERISTICS (MOC)

The MOC technique was implemented in the U.S. Geological Survey two-dimensional transport model (Konikow and Bredehoeft, 1978), and has been widely used in field studies. The method of characteristics uses a conventional particle tracking technique for solving the advection term. At the beginning of the simulation, a set of moving particles is distributed in the flow field either randomly or with a fixed pattern. A concentration and a position in the Cartesian coordinate system are associated with each of these particles. Particles are tracked forward through the flow field using a small time increment. At the end of each time increment, the average concentration at cell *m* due to advection alone over the time increment, or $C_m^{n^*}$, is evaluated from the concentrations of moving particles which happen to be located within cell *m*. T'his is expressed in the following equation (also see Fig. 3. 1):

$$C_m^{n^*} = \frac{1}{NP} \sum_{l=1}^{NP} C_l^n \qquad (3.6)$$

where

*NP* is the number of particles within cell *m;*

$C_l^n$ is the concentration of the $l^{th}$ particle at time level *n*;

After completing the evaluation of $C_m^{n^*}$ for all cells, a weighted concentration, $C_m^{\hat{n}}$, is calculated based on $C_m^{n^*}$ and the concentration at the old time level $C_m{}^n$.

$$C_m^{\hat{n}} = \omega C_m^{n^*} + (1-\omega)C_m^n \qquad (3.7)$$

Fig. 3.1. Illustration of the Method Of Characteristics (MOC). A set of moving particles are tracked forward during each time period. An intermediate concentration, equal to the average of the concentrations of all particles in the cell, is assigned to each cell. This intermediate concentration accounts for the effect of advection during the period since the preceding time level, and is used to calculate changes in concentration due to dispersion and other processes over that period.

where T is a weighting factor between 0 and 1. $C_m^{\hat{n}}$ is then used to calculate the second term in equation (3.5), or the changes in concentration due to dispersion, sink/source mixing, and chemical reactions (the terms on the right-hand side of equation 3.3) with an explicit finite difference method, i.e.,

$$\Delta C_m^{n+1} = \Delta t \times RHS(C_m^{\hat{n}}) \qquad (3.8)$$

The use of the weighted concentration in equation (3.8) represents an averaged approach because the precesses of dispersion, sink/source mixing, and/or chemical reactions occur throughout the time increment.

The concentration for cell *m* at the new time level *(n+1)* is then the sum of the $C_m^{n^*}$ and $\Delta C_m^{n+1}$ terms. The concentrations of all moving particles are also updated to reflect the change due to dispersion, sink/source mixing, and chemical reactions. This completes the calculation of one transport step for the method of characteristics. The procedure is repeated until the end of a desired time period is reached.

One of the most desirable features of the MOC technique is that it is virtually free of numerical dispersion, which creates serious difficulty in many standard numerical schemes. The major drawback of the MOC technique is that it can be slow and requires a large amount of computer memory when it is necessary to track a large number of moving particles, especially in three dimensions. The MOC technique can also lead to large mass balance discrepancies under certain situations because the MOC technique, like other mixed Eulerian-Lagrangian solution techniques, is not entirely based on the principle of mass conservation. In the MT3D transport model, the computer memory requirement for the MOC technique is dramatically reduced through the use of a dynamic approach for particle distribution. The mass balance discrepancy problem is also overcome to a large extent through the use of consistent velocity interpolation schemes and higher-order particle tracking algorithms. Further discussion of these topics is given in the next chapter.

## 3.3 MODIFIED METHOD OF CHARACTERISTICS (MMOC)

The modified method of characteristics was originally developed to approximate the advection term accurately without sacrificing a great deal of computational efficiency (e.g., Russell and Wheeler, 1983; Cheng et. al., 1984). The MMOC technique is similar to the MOC technique except in the treatment of the advection term. Unlike the MOC technique, which tracks a large number of moving particles forward in time and keeps track of the concentration and position of each particle, the MMOC technique places one fictitious particle at the nodal point of the fixed grid at each new time level *(n+l)*. The particle is tracked backward to find its position at the old time level *(n)*. The concentration associated with that position is used to approximate the $C_m^{n^*}$ term (also see Fig. 3.2):

$$C_m^{n^*} = C^n(x_p) = C^n(x_m - \boldsymbol{d}) \tag{3.9}$$

where

$x_p$ is the position which a particle starting from nodal point m reaches when it is tracked backward along the reverse pathline over the time increment ) *t;*

$x_m$ is the position vector of nodal point *m*;

*d* is the characteristic nodal displacement, or the distance along a particle path from $x_m$ to $x_p$;

$C^n(x_p)$ is the concentration at position $x_p$ at the old time level *(n)*. It is generally interpolated from concentrations at neighboring nodal points.

The MMOC technique uses one particle for each finite-difference cell, whereas the MOC technique generally requires several particles per cell. Therefore, the MMOC technique, used in conjunction with a simple lower-order interpolation scheme, is normally faster than the MOC technique. Furthermore, because the MMOC technique starts particles at nodal points at each new time level, there is no need to store the particle identities in computer memory. Hence, for problems in which the MOC technique requires a large number of particles, the MMOC technique requires much less computer memory. The MMOC technique is also free of artificial oscillations if implemented with a lower-order interpolation scheme such as linear interpolation (also referred to as bilinear in two dimensions or trilinear in three dimensions). However, with a lower-order interpolation scheme, the MMOC technique introduces some numerical dispersion, especially for sharp front problems. Higher-order interpolation schemes can be used to eliminate or reduce numerical dispersion. For example, Cheng et. al. (1984) used a quadratic interpolation scheme in two-dimensional simulations and pointed out that it is free of numerical dispersion. However, it is computationally less efficient than the linear scheme and can lead to severe artificial oscillations for sharp front problems (e.g., Fig. 2. lb in Chapter 2). Healy and Russell (1989) tested several interpolation schemes for one-dimensional problems and concluded that a mixed linear/quadratic scheme can minimize both numerical dispersion and artificial oscillations. However, it requires much more computational work in a multi-dimensional simulation than the linear scheme and does not conserve mass as well, thereby offsetting much of the advantage of the MMOC technique.

Fig. 3.2. Illustration of theModified Method Of Characteristics (MMOC). One fictitious particle is placed at each node and tracked backward in time to find its position at the previous time level. The concentration associated with that position is the intermediate concentration due to the effect of advection during the period since the preceding time level.

For these reasons, the MMOC technique in the MT3D transport model is implemented only with a lower-order interpolation scheme and is intended for use in situations where sharp fronts are not present, so that any numerical dispersion error resulting from the solution scheme is insignificant.

## 3.4 HYBRID METHOD OF CHARACTERISTICS (HMOC)

As shown in the preceding discussions, either the MOC or the MMOC scheme may be utilized to solve the mixed Eulerian-Lagrangian equation. The selection of the method is based on such considerations as field conditions (whether the concentration field has sharp or smooth fronts) and computer resources available (generally the MOC solution requires more memory space and longer execution time). A third option is to use a hybrid of the two methods; this option is referred to here as the hybrid method of characteristics (HMOC).

The HMOC technique attempts to combine the strengths of the MOC and the MMOC techniques by using an automatic adaptive scheme conceptually similar to the one proposed by Neuman (1984). The fundamental idea behind this scheme is automatic adaptation of the solution process to the nature of the concentration field. When sharp concentration fronts are present, the advection term is solved by the MOC technique through the use of moving particles dynamically distributed around each front. Away from such fronts, the advection term is solved by the MMOC technique with fictitious particles placed at the nodal points directly tracked backward in time. When a front dissipates due to dispersion and chemical reactions, the forward tracidng stops automatically and the corresponding particles are removed. By selecting an appropriate criterion for controlling the switch between the MOC and MMOC schemes, the adaptive procedure can provide accurate solutions to transport problems over the entire range of Peclet numbers fiom 0 to4 with virtually no numerical dispersion, while at the same time using far fewer particles than would be required by the MOC scheme alone.

Under certain circumstances, the choice for the adaptive criterion used in the HMOC scheme may not be obvious and the adaptive procedure may not lead to an optimal solution. In these cases, manual selection of either the MOC or the MMOC scheme may be more efficient. Therefore, all of the these three solution schemes are included in the current version of the MT3D transport model.

# Chapter 4
# NUMERICAL IMPLEMENTATION

## 4.1 SPATIAL DISCRETIZATION

The MT3D transport model follows the same spatial discretization convention as used by the U. S. Geological Survey modular three-dimensional finite-difference groundwater flow model, referred to as MODFLOW (McDonald and Harbaugh, 1988). An aquifer system is discretized into a mesh of blocks, or cells, the locations of which are described in terms of rows (1), columns (J), and layers (K) as illustrated in Fig. 4.l. Following the convention used in Fig. 4.1, the width of cells in the row direction, at a given column, J, is designated )$r_j$ **,** the width of cells in the column direction, at a given row, I, is designated )$c_i$ , and the thickness of cells in a given layer, K, is designated )$v_k$ . Thus a cell with indices (i,j,k) has a volume of )$r_j$ , )$c_i$ , )$v_k$ .

While the flow model does not require the designation of x, y, and z coordinate axes, the transport model does. In the MT3D model, an assumption is made that the x, y, and z coordinate axes are oriented along the row, column, and layer directions, respectively. The origin of the Cartesian coordinate system is located at the upper, top, left corner of the cell at the first row, first column, and first layer, or cell (1,1,1), as illustrated in Fig. 4.2. Because the convention followed in both the MT3D and MODFLOW models is to number layers from the top down, the z axis is pointed downward in the direction of decreasing elevation. With the Cartesian coordinate system, )$r_j$ along the row direction is equivalent to )$x_j$ along the x axis; )$c_i$ along the column direction is equivalent to )$y_i$ along the y axis; and )$v_k$ along the layer direction is equivalent to )$z_k$ along the z axis.

The fixed grid system of the transport model is based on the block-centered formulation as illustrated in Fig. 4.3. The block-centered formulation places a point, called a node, at the center of the cell, where the concentration or hydraulic head is calculated. The chemical and hydraulic parameters such as dispersivities or hydraulic conductivities are assumed to be uniform over the extent of a cell.

Fig. 4.1. Spatial discretization of an aquifer system(afterMcDonald and Harbaugh,1988).

Fig. 4.2. Cartesian coordinate system used in the MT3D transport model.

Fig. 4.3. Diagram showing the block-centered grid system (after McDonald and Harbaugh, 1988).

As shown in Figs. 4.1. and 4.2, an aquifer system is normally divided areally by two sets of parallel, orthogonal lines, and vertically by parallel, horizontal planes so that each cell formed by the discretization is a rectangular block. To allow flexibility in handling geologic units of varying thickness, the MT3D transport model, as in MODFLOW, permits the use of a deformed mesh in the vertical direction as illustrated in Fig. 4.4. The deformed vertical discretization, however, can introduce some numerical discretization error, especially in the transport simulation. Therefore, when the MT3D model is used with highly deformed vertical discretization, the simulation results should be evaluated carefully to ensure their accuracy.

## 4.2 TEMPORAL DISCRETIZATION

In most flow models, such as MODFLOW, simulation time is usually divided into "stress periods" -- time intervals during which all external stress parameters (i.e., sink/source) are constant. Stress periods are, in turn, divided into time steps, if the simulation is transient. The time steps within each stress period usually form a geometric progression. The length of each step is normally calculated by the program using the user-specified length of the stress the number of time steps and a time-step multiplier.

In the MT3D model, simulation is based on the implicit head solution provided by a separate flow model, and the explicit transport solution based on the mixed Eulerian-Lagrangian schemes. Thus, the length of the time step used for the head solution may be too large for the transport solution, because the explicit transport solution has certain stability criteria associated with it. Each time step of the head solution is, therefore, divided further into smaller time increments, called transport steps, during which heads are considered constant. The length of each transport step can be specified in the model input, or determined by the model with an automatic stepsize control procedure. The discretization of time is illustrated in Fig. 4.5.

Fig. 4.4. Schemes of vertical discretization (afterMcDonald and Harbaugh,1988).

Fig. 4.5. Discretization of simulation time in the transport model.

## 4.3 EVALUATION OF THE ADVECTION TERM

### 4.3.1 Velocity Interpolation

Both the method of characteristics and the modified method of characteristics involve the use of a particle tracking technique to approximate the advective component of the transport process. Since any particle tracking technique requires the evaluation of velocity at an arbitrary point from hydraulic heads calculated at nodal points, it is necessary to use a velocity interpolation scheme in the particle tracking calculations.

The velocity interpolation scheme used in this transport model is simple piecewise linear interpolation (e.g., Pollock, 1988; Zheng, 1988). This scheme assumes that a velocity component varies linearly within a finite-difference cell with respect to the direction of that component. Thus, the x-component of the Darcy velocity at an arbitrary point within a cell (i,j,k) can be expressed in terms of the fluxes on cell interfaces in the same direction (Fig. 4.6):

$$q_x(x_p,y_p,z_p) = (1-\alpha_x)\,q_{i,j-1/2,k} + \alpha_x q_{i,j+1/2,k} \tag{4.1}$$

where

$q_{i,j-1/2,k} = -K_{i,j-1/2,k}\dfrac{(h_{i,j,k}-h_{i,j-1,k})}{x_j - x_{j-1}}$, is the flux, or the specific discharge, through the interface between cells (i,j-l,k) and (i,j,k), and $K_{i,,j-1/2,k}$ is the harmonic mean of hydraulic conductivity between the two cells. The flux at the cell interface is calculated in the flow model and directly used in the transport model;

$q_{i,j+1/2,k} = -K_{i,j+1/2,k}\dfrac{(h_{i,j+1,k}-h_{i,j,k})}{x_{j+1} - x_j}$ is the flux through the interface between cells

(i,j,k) and (i,j+l,k);

$\alpha_x = \dfrac{x_p - x_{j-1/2}}{\Delta x_j}$ is the linear interpolation factor for the x component;

$x_p$, $y_p$, $z_p$, are the Cartesian coordinates of the particle location;

$x_{j\mp 1/2}$ is the x coordinates of the left and right interfaces of the cell (i,j,k);

$x_j$ is the x coordinates of the node (i,j,k); and

) $x_j$ is the cell width along the x-axis at cell (i,j,)

Fig. 4.6. The velocity interpolation scheme used in particle tracking.

The x-component of the linear or pore water velocity, $v_x$, is then obtained from:

$$v_x(x_p, y_p, z_p) = \frac{q_x(x_p, y_p, z_p)}{\theta_{i,j,k}} \tag{4.2}$$

where $2_{i,\,j,k}$ is the porosity value at cell (i,j,k).

Similarly, the y- and z- components of the velocity are calculated as:

$$q_y(x_p, y_p, z_p) = (1 - \alpha_y) q_{i-1/2,j,k} + \alpha_y q_{i+1/2,j,k} \tag{4.3}$$

$$v_y(x_p, y_p, z_p) = \frac{q_y(x_p, y_p, z_p)}{\theta_{i,j,k}} \tag{4.4}$$

where $\alpha_y = \frac{y_p - y_{i-1/2}}{\Delta y_i}$ is the linear interpolation factor for the y-component; and

$$q_z(x_p, y_p, z_p) = (1 - \alpha_z) q_{i,j,k-1/2} + \alpha_z q_{i,j,k+1/2} \tag{4.5}$$

$$v_z(x_p, y_p, z_p) = \frac{q_z(x_p, y_p, z_p)}{\theta_{i,j,k}} \tag{4.6}$$

where $\alpha_z = \frac{z_p - z_{k-1/2}}{\Delta z_k}$ is the linear interpolation factor for the z- component.

The velocity field generated with this scheme is consistent with the block-centered finite-difference formulation of the three-dimensional flow equation, and thus conserves mass locally within each finite-difference block. It also preserves the velocity discontinuities caused by changes in hydraulic conductivities present in heterogeneous media.

It is noted that this velocity scheme differs from the multi-linear scheme used in earlier method-of-characteristics models (e.g., Garder et. al., 1964; Konikow and Bredehoeft, 1978). The multi-linear scheme in a three-dimensional flow field assumes that velocity components vary linearly in all three directions, and thus generates a continuous velocity field in every direction. Goode (1990) notes that the multi-linear scheme may result in more satisfactory results in homogeneous media. However, the multi-linear scheme is not consistent with the cell-by-cell mass balance described by the block-centered finite-difference formulation and does not preserve the velocity discontinuities present in heterogeneous media, unlike the piecewise linear scheme. Because of this and because the piecewise linear scheme is computationally much more efficient, the piecewise linear scheme has been utilized in the MT3D model.

### 4.3.2 Particle Tracking

With the velocity field known, a numerical tracking scheme can be used to move particles from one position to another to approximate the advection of the contaminant front. Traditionally, the first-order Euler algorithm has been used for particle tracking (e.g., Konikow and Bredehoeft, 1978):

$$\begin{cases} x^{n+1} = x^{n} + \dfrac{\Delta t}{R} v_x(x^{n}, y^{n}, z^{n}) \\ y^{n+1} = y^{n} + \dfrac{\Delta t}{R} v_y(x^{n}, y^{n}, z^{n}) \\ z^{n+1} = z^{n} + \dfrac{\Delta t}{R} v_z(x^{n}, y^{n}, z^{n}) \end{cases} \tag{4.7}$$

where $x^{n+1}$, $y^{n+1}$, $z^{n+1}$ are the particle coordinates at the new time level $(n+1)$; $x^n$, $y^n$, $z^n$ are the coordinates at the old time level $(n)$; $v_x$, $v_y$, $v_z$, are the linear velocities evaluated at $(x^n, y^n, z^n)$; and $R$ is the retardation factor resulting from the incorporation of sorption isotherms into the transport equation. ) t is the size of the transport step, which is generally determined from the so-called "Courant condition", or,

$$|\Delta t| \le \gamma_c R\, MIN \left( \frac{\Delta t}{v_x}, \frac{\Delta t}{v_y}, \frac{\Delta t}{v_z} \right) \tag{4.8}$$

where $(_c$ , is the Courant number, representing the number of cells a particle will be allowed to move in any direction in one transport step. The particle tracking is forward if the sign of ) *t* is positive, and backward if the sign of ) *t* is negative.

A uniform step size, ) *t,* is used for all moving particles during each transport step in the particle tracking calculations. For particles located in areas of relatively uniform velocity, the first-order Euler algorithm may have sufficient accuracy. However, for particles located in areas of strongly converging or diverging flows, for example, near sources or sinks, the first--order algorithm may not be sufficiently accurate, unless ) *t* is very small. In these cases a higher-order algorithm such as the fourth-order Runge-Kutta method may be used (e.g., Zheng, 1988). The basic idea of the fourth-order Runge-Kutta method is to evaluate the velocity four times for each tracking step: once at the initial point, twice at two trial midpoints, and once at a trial end point (Fig. 4.7). A weighted velocity based on values evaluated at these four points is used to move the particle to the new position ( $x^{n+1}$, $y^{n+1}$, $z^{n+1}$). This process may be expressed as follows:

$$\begin{cases} x^{n+1} = x^n + \dfrac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \\ y^{n+1} = y^n + \dfrac{1}{6}(l_1 + 2l_2 + 2l_3 + l_4) \\ z^{n+1} = z^n + \dfrac{1}{6}(m_1 + 2m_2 + 2m_3 + m_4) \end{cases} \qquad (4.9)$$

where

$$\begin{aligned} k_1 &= \Delta t v_x(x^n, y^n, z^n, t^n) \\ k_2 &= \Delta t v_x(x^n + k_1/2, y^n + l_1/2, z^n + m_1/2, t^n + \Delta t/2) \\ k_3 &= \Delta t v_x(x^n + k_2/2, y^n + l_2/2, z^n + m_2/2, t^n + \Delta t/2) \\ k_4 &= \Delta t v_x(x^n + k_3, y^n + l_3, z^n + m_3, t^n + \Delta t) \end{aligned}$$

$$\begin{aligned} l_1 &= \Delta t v_y(x^n, y^n, z^n, t^n) \\ l_2 &= \Delta t v_y(x^n + k_1/2, y^n + l_1/2, z^n + m_1/2, t^n + \Delta t/2) \\ l_3 &= \Delta t v_y(x^n + k_2/2, y^n + l_2/2, z^n + m_2/2, t^n + \Delta t/2) \\ l_4 &= \Delta t v_y(x^n + k_3, y^n + l_3, z^n + m_3, t^n + \Delta t) \end{aligned}$$

$$\begin{aligned} m_1 &= \Delta t v_z(x^n, y^n, z^n, t^n) \\ m_2 &= \Delta t v_z(x^n + k_1/2, y^n + l_1/2, z^n + m_1/2, t^n + \Delta t/2) \\ m_3 &= \Delta t v_z(x^n + k_2/2, y^n + l_2/2, z^n + m_2/2, t^n + \Delta t/2) \\ m_4 &= \Delta t v_z(x^n + k_3, y^n + l_3, z^n + m_3, t^n + \Delta t) \end{aligned}$$

Fig. 4.7. The fourth-order Runge-Kutta method. In each step, the velocity is evaluated four times: once at the initial point, twice at trial midpoints, and once at a trial endpoint. From these velocities a weighted velocity is calculated which is used to compute the final position of the particle (shown as a filled dot). (Modified from Press el. al., 1986).

The fourth-order Runge-Kutta algorithm is more accurate and permits the use of larger tracking steps. However, the computational effort required by the fourth-order Runge-Kutta algorithm is considerably more than that required by the Euler algorithm, making the former less efficient than the latter for three-dimensional simulations when a very large number of particles are used. For these reasons, the MT3D model provides three options: a first-order Euler algorithm, a fourth-order Runge-Kutta algorithm, and a combination of these two. These options, when used properly, allow sufficient accuracy throughout the finite-difference grid without using exceedingly small stepsizes.

### 4.3.3 The MOC Procedure

The first step in the method of characteristics is to generate representative particles in the finite-difference grid. Instead of placing a uniform number of particles in every cell of the grid, a dynamic approach is used in the MT3D transport model to control the distribution of moving particles. The number of particles placed at each cell is normally set either at a high level or at a low level, according to the so-called "relative cell concentration gradient", or, DCCELL, defined as:

$$DCCELL_{i,j,k} = \frac{CMAX_{i,j,k} - CMIN_{i,j,k}}{CMAX - CMIN} \qquad (4.10)$$

where

$CMAX_{i,j,k} = \max\limits_{kk=k-1}^{k+1}\left(\max\limits_{jj=j-1}^{j+1}\left(\max\limits_{ii=i-1}^{i+1}\left(C_{ii,jj,kk}\right)\right)\right)$ , is the maximum concentration in the immediate vicinity of the cell (i,j,k);

$CMIN_{i,j,k} = \min\limits_{kk=k-1}^{k+1}\left(\min\limits_{jj=j-1}^{j+1}\left(\min\limits_{ii=i-1}^{i+1}\left(C_{ii,jj,kk}\right)\right)\right)$ , is the minimum concentration in the immediate vicinity of the cell (ijk);

*CMAX* is the maximum concentration in the entire grid; and

*CMIIV* is the minimum concentration in the entire grid.

With the dynamic approach, the user defines the criterion, DCEPS, which is a small integer number near zero; the higher number of particles, NPH, is placed in cells where the relative concentration gradient is greater than DCEPS, and the lower number of particles, NPL, in cells where the relative concentration gradient is less than DCEPS, i.e.,

$$\begin{cases} NP_{i,j,k} = NPH\,, & \text{if } DCCELL_{i,j,k} > DCEPS\ ; \\ NP_{i,j,k} = NPL\,, & \text{if } DCCELL_{i,j,k} \le DCEPS \end{cases} \tag{4.11}$$

where *NPi,j,k* is number of particles placed in cell (i,j,k).

Initially, if the concentration gradient at a cell is zero or small, (i.e., the concentration field is relatively constant near that cell), the number of particles placed in that cell is NPL, which may be zero or some small integer number, this is done because the concentration change due to advection between that cell and the neighboring cells will be insignificant. If the concentration gradient at a cell is large, which indicates that the concentration field near that cell is rapidly changing, then the number of particles placed in that cell is NPH.

As particles leave source cells or accumulate at sink cells, it becomes necessary to insert new particles at sources, or remove particles at sinks. At non-source or non-sink cells, it also becomes necessary to insert or remove particles as the cell concentration gradient changes with time. This is done in the dynamic insertion-deletion procedure by specifying the minimum and maximum numbers of particles allowed per cell, called NPMIN and NPMAX, respectively. When the number of particles in any cell, (source or non-source), becomes smaller than the specified minimum, or NPMIN, new particles equal to NPL or NPH are inserted into that cell without affecting the existing particles. On the other hand, when the number of particle in any cell, (sink or non-sink), exceeds the specified maximum, or NP , particles are removed from that cell until the maximum is met. To save computer storage, memory space occupied by the deleted particles is reused by newly inserted particles.

Fig. 4.8. Comparison of the uniform and dynamic appoaches in controlling the distribution of moving particles.

Fig. 4.8 illustrates the dynamic particle distribution approach in contrast with the uniform approach in simulating two-dimensional solute transport from a continuous point source in a uniform flow field. Whereas the uniform approach inserts and maintains an approximately uniform particle distribution throughout the simulated domain, the dynamic approach adjusts the distribution of moving particles dynamically, adapting to the changing nature of the concentration field. In many practical problems involving contaminant transport modeling, the contaminant plumes may occupy only a small fraction of the finite-difference grid and the concentrations may be changing rapidly only at sharp fronts. In these cases, the number of total particles used is much smaller than that required in the uniform particle distribution approach, thereby dramatically increasing the efficiency of the method-of-characteristics model with little loss in accuracy.

Particles can be distributed either with a fixed pattern or randomly, as controlled by the user-specified option (see Fig. 4.9). If the fixed pattern is chosen, the user determines not only the number of particles to be placed per cell, but also the pattern of the particle placement in plan view and the number of vertical planes on which particles are placed within each cell block.  If the random pattern is chosen, the user only needs to specify the number of particles to be placed per cell.  The program then calls a random number generator and distributes the required number of particles randomly within each cell block. (The selection of these options is discussed in Chapter 6: Input Instructions).  The fixed pattern may work better if the flow field is relatively uniform.  On the other hand, if the flow field is highly nonuniform with many sinks or sources in largely heterogeneous media, the random pattern may capture the essence of the flow field better than the fixed pattern does.

Fig. 4.9. Initial placement of moving particles.

Each particle is associated with a set of attributes, that is, the x-, y-, and z-coordinates and the concentration.  The initial concentration of the particle is assigned as the concentration of the cell where the particle is initialized.  At the beginning of each transport step, all particles are moved over the time increment, At, using the particle tracking techniques described previously.  The x-, y-, and z-coordinates of the moving particles are then updated to reflect their new positions at the end of the transport step.  The average concentration of a finite-difference cell at the end of the transport step due to advection alone, $C^{n^*}_{i,j,k}$ , is obtained by accumulating the concentrations of all particles that are located at that cell, divided by the number of particles:

$$C^{n^*}_{i,j,k} = \frac{1}{NP_{i,j,k}} \sum_{l=1}^{NP_{i,j,k}} C^{n}_{l}, \qquad if\ NP_{i,j,k} > 0 \tag{4.12}$$

If the number of particles at the cell is zero, then the average concentration after particle tracking is set equal to the cell concentration at the previous time level because the concentration change at that cell over the time increment is either negligible or dominated by an external source:

$$C^{n^*}_{i,j,k} = C^{n}_{i,j,k}, \qquad if\ NP_{i,j,k} = 0 \tag{4.13}$$

It is necessary to locate the cell indices of any particle in the tracking and averaging calculations as described above. If the finite-difference grid is regular, it is straightforward to convert particle coordinates *($x_p$, $y_p$, $z_p$,)* to cell indices *(JP, IP, KP)* according to the following formulas:

$$\begin{cases} JP = INT\ (x_p/\Delta x) + 1 \\ IP = INT\ (y_p/\Delta y) + 1 \\ KP = INT\ (z_p/\Delta z) + 1 \end{cases} \qquad (4.14)$$

where *INT(X)* is a FORTRAN function, equal to the truncated value of x; and )*x*, )*y*, )*z* are the uniform grid spacings along the x-, y-, and z-axes. If the finite-difference grid is irregular, then, an efficient bisection routine is used to locate the cell indices from the x-, y-, and z-coordinates as illustrated in Fig. 4. 1 0.

Fig.4.10. To determine in which cell a particle P is located in an irregular mesh, a searching procedure is first started from a guessed position, either up or down, in increments of one, two, then four, etc., until the desired value is bracketed. Second, a bisection routine is used to bisect the nodal points in the immediate vicinity of the particle position, JLO and JHI. Finally, the coordinate of the particle is compared with that of the interface between JLO and JHI to find out whether P is located in cell JW or cell JHI. In this example, if the guessed position were J = 7 instead of J = 2, the cell index of P would have been located in far fewer steps. In the particle tracking calculations, the next particle to be moved is usually adjacent to the particle that has just been moved; thus the cell indices of the particle just moved are used as the guessed indices for the particle to be moved next.

After the $C^{n^*}_{i,j,k}$ term is evaluated at every cell, it is used to calculate the concentration change due to dispersion, sink/source mixing and/or chemical reactions ( $\Delta C^{n+1}_{i,j,k}$ ) using the finite-difference method as discussed in Sections 4.4, 4.5 and 4.6. The concentration of all active particles is then updated by adding the concentration change ( $\Delta C^{n+1}_{i,j,k}$ ) Calculated at the cell where each particle is located. Therefore, for moving particles located at cell (*i,j,k*):

$$C_l^{n+1} = C_l^n + \Delta C_{i,j,k}^{n+1} \qquad (4.15)$$

where $C_l^{n+1}$ is the concentration of the $l^{th}$ particle which is located at cell (i,j,k) at the new time level. If ) $\Delta C_{i,j,k}^{n+1}$ is positive, equation (4.15) is applied directly. However, if $\Delta C_{i,j,k}^{n+1}$ is negative, the concentration of the moving particle may become negative if its concentration at the old time level, $C_l^n$, is zero or small. To prevent this from happening, a weighting procedure, similar to the one used in Konikow and Bredehoeft (1978), is implemented which places more weight on particles with higher concentrations than particles with lower concentrations in the same cell:

$$C_l^{n+1} = C_l^n \times \left( \frac{1 + \Delta C_{i,j,k}^{n+1}}{C_{i,j,k}^{n^*}} \right) \qquad (4.16)$$

### 4.3.4 The MMOC Procedure

The first step in the MMOC procedure is to move a particle located at the nodal point of the cell backward in time using the particle tracking techniques. The purpose of this backward tracking is to find the position from which a particle would have originated at the beginning of the time step so as to reach the nodal point at the end of the time step. The concentration associated withe that position, denoted as $(\hat{x},\hat{y},\hat{z})$ is the concentration of the cell due to advection alone over the time increment ) *t.*

The position $(\hat{x},\hat{y},\hat{z})$ generally does not coincide with a nodal point. Thus, it is necessary to interpolate the concentration at $(\hat{x},\hat{y},\hat{z})$ from concentrations at neighboring nodal points. The interpolation scheme used in the MT3D transport model is first-order polynomial interpolation, also referred to as bilinear in two dimensions or trilinear in three dimensions. The general equation for first-order polynomial interpolation is as follows, assuming that $\hat{x}$ is located between nodes $X_{j-1}$ and $x_j$, between $\hat{y}$, and $y_{i-1}$, and $\hat{z}$ between $z_{k-1}$, and $z_k$ (also see Fig. 4.1 1):

$$\begin{aligned} C(\hat{x},\hat{y},\hat{z}) = {} & (1-\omega_x)(1-\omega_y)(1-\omega_z)C_{i-1,j-1,k-1} + (1-\omega_x)\,\omega_y(1-\omega_z)\,C_{i,j-1,k-1} \\ & + \omega_x(1-\omega_y)\,(1-\omega_z)C_{i-1,j,k-1} + \omega_x\,\omega_y(1-\omega_z)C_{i,j,k-1} \\ & + (1-\omega_x)(1-\omega_y)\omega_z C_{i-1,j-1,k} + (1-\omega_x)\omega_y\omega_z C_{i,j-1,k} \\ & + \omega_x(1-\omega_y)\,\omega_z C_{i-1,j,k} + \omega_x\omega_y\omega_z C_{i,j,k} \end{aligned} \qquad (4.17)$$

where $T_x$, $T_y$, and $T_z$ are interpolation factors as given below:

$$\begin{cases} \omega_x = \dfrac{\hat{x} - x_{j-1}}{0.5\Delta x_j + 0.5\Delta x_{j-1}} \\ \omega_y = \dfrac{\hat{y} - y_{i-1}}{0.5\Delta y_i + 0.5\Delta y_{i-1}} \\ \omega_z = \dfrac{\hat{z} - z_{k-1}}{0.5\Delta z_k + 0.5\Delta z_{k-1}} \end{cases} \qquad (4.18)$$

If the x-, y-, or z-dimension is not simulated, the weighting factor in the respective direction is zero. If any cell is inactive, the cell is skipped in the calculation. The low-order interpolation represented by equation (4.17) is computationally very efficient and has small mass balance error. It is also virtually free of artificial oscillation. However, this linear scheme does not eliminate numerical dispersion. As the concentration fronts become sharper, the amount of numerical dispersion increases. However, in the MT3D transport model, the MMOC scheme is only intended for problems with relatively smooth concentration fronts (sharp front problems are handled by the MOC technique). When the concentration field is relatively smooth, the numerical dispersion resulting from the MMOC technique is insignificant.

Fig. 4.11 Interpolation of the concentration at point P from the concentrations at neighboring nodes using the trilinear scheme in three dimensions.

Sinks or sources create special problems for the MMOC scheme, and thus have to be treated differently. First, examine a sink cell with inward hydraulic gradients on all of the cell interfaces as illustrated in Fig. 4.12. If the sink is symmetric, the velocity at the nodal point is zero. Therefore, instead of placing one particle at the nodal point, the MT3D program places multiple particles within the cell. The number and distribution of these particles are controlled by the user-specified options in a manner similar to those described in the MOC procedure. Each particle is tracked backward over ) *t*, and its concentration is interpolated for neighboring nodes. The cell concentration is then averaged from the concentrations of all particles, based on the reverse distance algorithm:

$$C_{i,j,k}^{n*} = \frac{\displaystyle\sum_{l=1}^{NP} \frac{C_l^n}{d_l}}{\displaystyle\sum_{l=1}^{NP} \frac{1}{d_l}} \qquad (4.19)$$

where $d_l$ is the distance between the nodal point and the position where the $l^{th}$ particle is initially placed. The reverse distance algorithm differs from the simple average algorithm used in the MOC scheme, in that the former gives more weight to particles that are located closer to the node whereas the latter gives the same weight to all particles in the same cell.

Next, consider a source cell with outward hydraulic gradients on all cell interfaces. Backward tracking will cause particles placed in the source cell to converge toward the nodal point so that:

$$C_{i,j,k}^{n^*} = C_{i,j,k}^{n} \tag{4.20}$$

With the MMOC scheme, particles are restarted at each time step, and thus, there is no need to store the particle locations and concentrations in computer memory. Thus, the MMOC solution normally requires far less computer memory, and is generally more efficient computationally than the MOC solution.

(a) At a sink cell with inward gradients on all interfaces

(b) Instead of placing one single particle at the node, multiple particles are placed and tracked backward. In this example, 8 particles distributed with a fixed pattern are used. However, both the number and the pattern can be changed in the user-specified options.

Fig. 4.12. Special treatment of sink cells in the MMOC scheme.

### 4.3.5 The HMOC Procedure

The forward-tracking MOC scheme is uniquely suitable for sharp front problems (pure advection or largely advection-dominated problems) because it virtually eliminates numerical dispersion, a serious problem plaguing many standard numerical procedures. The MOC scheme implemented with dynamic particle distribution is also very efficient computationally for many practical problems where the contaminant plume occupies only a small fraction of the finite-difference grid, and the concentration field is changing rapidly only at sharp fronts. However, as the degree of advection domination over dispersion and chemical reactions decreases, the advantage of the MOC scheme is less obvious because as physical dispersion increases, numerical dispersion becomes less of a problem. Furthermore, as large physical dispersion causes the contaminant plume to spread through a large portion of the simulated domain, the number of moving particles needed by the MOC scheme can become very large for a three-dimensional simulation, pushing the memory requirement beyond the limits of many personal computers. The backward-tracking MMOC scheme tends to complement the MOC scheme for smooth front problems because the MMOC scheme requires far less computer memory, is generally more efficient computationally and introduces very little numerical dispersion.

If the flow field and the dispersivity parameters are relatively constant, and the spatial discretization is fairly regular, it may be straightforward to select either the MOC or the MMOC scheme to be used in the simulation based on the mesh Peclet number:

$$P_e = \frac{|v_i| \Delta x_i}{D_{ii}} \tag{4.21}$$

where $|v_i|$ is the magnitude of the seepage velocity component; ) $x_i$ is the cell width along the *i* direction and $D_{ii}$ is the component of the dispersion coefficient with respect to that direction. The MOC scheme is suitable for problems with large mesh Peclet numbers while the MMOC scheme can be used for problems with small mesh Peclet numbers. As a rule of thumb, the MOC scheme may be used effectively for problems with a mesh Peclet number greater than 10 while the MMOC scheme may be used for problems with a mesh Peclet number smaller than 0.1 without introducing any significant amount of numerical dispersion. It should be pointed out that this rule of thumb is based on a limited number of numerical experiments and may not be true for all situations.

Under certain circumstances, the use of the MOC scheme alone may require too much computer memory and execution time while the use of the MMOC scheme may lead to noticeable numerical dispersion, so that neither provides a satisfactory solution. In these cases, a hybrid scheme combining the MOC and MMOC schemes (or HMOC) may work best. The fundamental idea behind the hybrid MOC/MMOC scheme is to combine the strengths of the MOC and the MMOC techniques by using an automatic adaptive procedure, which causes MOC to be used in areas of steep concentration gradients and MMOC to be used in areas of low concentration gradients. The automatic selection is based on the sharpness of the concentration fronts, measured by the relative concentration gradient between the cell being considered and its neighboring cells as defined in equation 4.10. The implementation of the hybrid scheme is through the use of a user-specified criterion *DCHMOC:*

$$\begin{cases} MOC \ \ is \ \ used, & if \ DCCELL_{i,j,k} \succ DCHMOC \\ MMOC \ \ is \ \ used, & if \ DCCELL_{i,j,k} \le DCHMOC \end{cases} \tag{4.22}$$

At the beginning of each transport step, the value of *DCCELL* calculated at each cell is compared to *DCHMOC.* If *DCCELL*$_{i,j,k,}$ > *DCHMOC,* the advection term at that cell is solved using the MOC technique with the aid of moving particles. If there are no particles present at that cell, new particles are inserted. On the other hand, if *DCCELL*$_{i,j,k}$ $\leq$ *DCHMOC,* the advection term at that cell is solved using the MMOC technique. If there are still particles present at that cell, these particles are removed. The *DCHMOC* criterion is empirical, but values between 0.001 and 0.01 have been found to be generally adequate for the test problems discussed in Chapter 7. By selecting an appropriate valve for *DCHMOC,* the adaptive procedure can provide accurate solutions to the transport problems over the entire range of mesh Peclet numbers from 0 to $\infty$ with virtually no numerical dispersion, while at the same time using far fewer moving particles than would be required by the MOC scheme alone.

## 4.4 EVALUATION OF THE DISPERSION TERM

After completing the evaluation of the cell concentration due to pure advection at the intermediate time level, or, $C^{n^*}_{i,j,k}$ , for all cells using the procedures described in Section 4.3, a weighted concentration, $C^{\hat{n}}_{i,j,k}$ , is calculated based on $C^{n^*}_{i,j,k}$ and the concentration at the old time level $C^{n}_{i,j,k}$:

$$C^{\hat{n}}_{i,j,k} = \omega C^{n^*}_{i,j,k} + (1+\omega) C^{n}_{i,j,k} \tag{4.23}$$

The weighted concentration $C^{\hat{n}}_{i,j,k}$ is then used to calculate the changes in concentration due to dispersion, sink/source mixing, and/or chemical reactions with the explicit finite-difference method. This is done because the processes of dispersion, sink/source mixing, and/or chemical reaction occur neither at the beginning of step, nor at the end of the step, but throughout the step. The weighted concentration, thus, represents an averaged approach.

The concentration change due to dispersion alone can be written as (see Section 3.1):

$$\begin{aligned}\frac{DC_{DSP}}{Dt} = \frac{1}{R}\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_i}\right) = \frac{1}{R}\Bigg[ & \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial x}\left(D_{xy}\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial x}\left(D_{xz}\frac{\partial C}{\partial z}\right) \\ & + \frac{\partial}{\partial y}\left(D_{yx}\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_{yy}\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial y}\left(D_{yz}\frac{\partial C}{\partial z}\right) \\ & + \frac{\partial}{\partial z}\left(D_{zx}\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial z}\left(D_{zy}\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_{zz}\frac{\partial C}{\partial z}\right)\Bigg]\end{aligned} \tag{4.24}$$

Equation 4.24 is solved with the fully explicit central finite-difference scheme. The finite difference equation for this scheme is given below:

$$
\begin{aligned}
\Delta C_{i,j,k}^{n+1} = \frac{\Delta t}{R_{i,j,k}^{n}} \Bigg\{ & D_{xx_{i,j+1/2,k}} \frac{C_{i,j+1,k}^{\hat{n}} - C_{i,j,k}^{\hat{n}}}{\Delta x_j (0.5\Delta x_j + 0.5\Delta x_{j+1})} - D_{xx_{i,j-1/2,k}} \frac{C_{i,j,k}^{\hat{n}} - C_{i,j-1,k}^{\hat{n}}}{\Delta x_j (0.5\Delta x_{j-1} + 0.5\Delta x_j)} \\
& + D_{xy_{i,j+1/2,k}} \frac{\omega_{x_{j+1/2}} C_{i+1,j,k}^{\hat{n}} + (1-\omega_{x_{j+1/2}}) C_{i+1,j+1,k}^{\hat{n}} - \omega_{x_{j+1/2}} C_{i-1,j,k}^{\hat{n}} - (1-\omega_{x_{j+1/2}}) C_{i-1,j+1,k}^{\hat{n}}}{\Delta x_j (0.5\Delta y_{i-1} + \Delta y_i + 0.5\Delta y_{i+1})} \\
& - D_{xy_{i,j-1/2,k}} \frac{\omega_{x_{j-1/2}} C_{i+1,j-1,k}^{\hat{n}} + (1-\omega_{x_{j-1/2}}) C_{i+1,j,k}^{\hat{n}} - \omega_{x_{j-1/2}} C_{i-1,j-1,k}^{\hat{n}} - (1-\omega_{x_{j-1/2}}) C_{i-1,j,k}^{\hat{n}}}{\Delta x_j (0.5\Delta y_{i-1} + \Delta y_i + 0.5\Delta y_{i+1})} \\
& + D_{xz_{i,j+1/2,k}} \frac{\omega_{x_{j+1/2}} C_{i,j,k+1}^{\hat{n}} + (1-\omega_{x_{j+1/2}}) C_{i,j+1,k+1}^{\hat{n}} - \omega_{x_{j+1/2}} C_{i,j,k-1}^{\hat{n}} - (1-\omega_{x_{j+1/2}}) C_{i,j+1,k-1}^{\hat{n}}}{\Delta x_j (0.5\Delta z_{k-1} + \Delta z_k + 0.5\Delta z_{k+1})} \\
& - D_{xz_{i,j-1/2,k}} \frac{\omega_{x_{j-1/2}} C_{i,j-1,k+1}^{\hat{n}} + (1-\omega_{x_{j-1/2}}) C_{i,j,k+1}^{\hat{n}} - \omega_{x_{j-1/2}} C_{i,j-1,k-1}^{\hat{n}} - (1-\omega_{x_{j-1/2}}) C_{i,j,k-1}^{\hat{n}}}{\Delta x_j (0.5\Delta z_{k-1} + \Delta z_k + 0.5\Delta z_{k+1})} \\
& + D_{yx_{i+1/2,j,k}} \frac{\omega_{y_{i+1/2}} C_{i,j+1,k}^{\hat{n}} + (1-\omega_{y_{i+1/2}}) C_{i+1,j+1,k}^{\hat{n}} - \omega_{y_{i+1/2}} C_{i,j-1,k}^{\hat{n}} - (1-\omega_{y_{i+1/2}}) C_{i+1,j-1,k}^{\hat{n}}}{\Delta y_i (0.5\Delta x_{j-1} + \Delta x_j + 0.5\Delta x_{j+1})} \\
& - D_{yx_{i-1/2,j,k}} \frac{\omega_{y_{i-1/2}} C_{i-1,j+1,k}^{\hat{n}} + (1-\omega_{y_{i-1/2}}) C_{i,j+1,k}^{\hat{n}} - \omega_{y_{i-1/2}} C_{i-1,j-1,k}^{\hat{n}} - (1-\omega_{y_{i-1/2}}) C_{i,j-1,k}^{\hat{n}}}{\Delta y_i (0.5\Delta x_{j-1} + \Delta x_j + 0.5\Delta x_{j+1})} \\
& + D_{yy_{i+1/2,j,k}} \frac{C_{i+1,j,k}^{\hat{n}} - C_{i,j,k}^{\hat{n}}}{\Delta y_i (0.5\Delta y_i + 0.5\Delta y_{i+1})} - D_{yy_{i-1/2,j,k}} \frac{C_{i,j,k}^{\hat{n}} - C_{i-1,j,k}^{\hat{n}}}{\Delta y_i (0.5\Delta y_{i-1} + 0.5\Delta y_i)} \\
& + D_{yz_{i+1/2,j,k}} \frac{\omega_{y_{i+1/2}} C_{i,j,k+1}^{\hat{n}} + (1-\omega_{y_{i+1/2}}) C_{i+1,j,k+1}^{\hat{n}} - \omega_{y_{i+1/2}} C_{i,j,k-1}^{\hat{n}} - (1-\omega_{y_{i+1/2}}) C_{i+1,j,k-1}^{\hat{n}}}{\Delta y_i (0.5\Delta z_{k-1} + \Delta z_k + 0.5\Delta z_{k+1})} \\
& - D_{yz_{i-1/2,j,k}} \frac{\omega_{y_{i-1/2}} C_{i-1,j,k+1}^{\hat{n}} + (1-\omega_{y_{i-1/2}}) C_{i,j,k+1}^{\hat{n}} - \omega_{y_{i-1/2}} C_{i-1,j,k-1}^{\hat{n}} - (1-\omega_{y_{i-1/2}}) C_{i,j,k-1}^{\hat{n}}}{\Delta y_i (0.5\Delta z_{k-1} + \Delta z_k + 0.5\Delta z_{k+1})} \\
& + D_{zx_{i,j,k+1/2}} \frac{\omega_{z_{k+1/2}} C_{i,j+1,k}^{\hat{n}} + (1-\omega_{z_{k+1/2}}) C_{i,j+1,k+1}^{\hat{n}} - \omega_{z_{k+1/2}} C_{i,j-1,k}^{\hat{n}} - (1-\omega_{z_{k+1/2}}) C_{i,j-1,k+1}^{\hat{n}}}{\Delta z_k (0.5\Delta x_{j-1} + \Delta x_j + 0.5\Delta x_{j+1})} \\
& - D_{zx_{i,j,k-1/2}} \frac{\omega_{z_{k-1/2}} C_{i,j+1,k-1}^{\hat{n}} + (1-\omega_{z_{k-1/2}}) C_{i,j+1,k}^{\hat{n}} - \omega_{z_{k-1/2}} C_{i,j-1,k-1}^{\hat{n}} - (1-\omega_{z_{k-1/2}}) C_{i,j-1,k}^{\hat{n}}}{\Delta z_k (0.5\Delta x_{j-1} + \Delta x_j + 0.5\Delta x_{j+1})} \\
& + D_{zy_{i,j,k+1/2}} \frac{\omega_{z_{k+1/2}} C_{i+1,j,k}^{\hat{n}} + (1-\omega_{z_{k+1/2}}) C_{i+1,j,k+1}^{\hat{n}} - \omega_{z_{k+1/2}} C_{i-1,j,k}^{\hat{n}} - (1-\omega_{z_{k+1/2}}) C_{i-1,j,k+1}^{\hat{n}}}{\Delta z_k (0.5\Delta y_{i-1} + \Delta y_i + 0.5\Delta y_{i+1})} \\
& + D_{zy_{i,j,k-1/2}} \frac{\omega_{z_{k-1/2}} C_{i+1,j,k-1}^{\hat{n}} + (1-\omega_{z_{k-1/2}}) C_{i+1,j,k}^{\hat{n}} - \omega_{z_{k-1/2}} C_{i-1,j,k-1}^{\hat{n}} - (1-\omega_{z_{k-1/2}}) C_{i-1,j,k}^{\hat{n}}}{\Delta z_k (0.5\Delta y_{i-1} + \Delta y_i + 0.5\Delta y_{i+1})} \\
& + D_{zz_{i,j,k+1/2}} \frac{C_{i,j,k+1}^{\hat{n}} - C_{i,j,k}^{\hat{n}}}{\Delta z_k (0.5\Delta z_k + 0.5\Delta z_{k+1})} - D_{zz_{i,j,k-1/2}} \frac{C_{i,j,k}^{\hat{n}} - C_{i,j,k-1}^{\hat{n}}}{\Delta z_k (0.5\Delta z_{k-1} + 0.5\Delta z_k)} \Bigg\} \qquad (4.25)
\end{aligned}
$$

where

$\Delta C_{DSP}^{n+1}$ is the concentration change due to dipersion from old time level *n* to new time level *n + 1*

$D_{xx}$, $D_{xy}$, $D_{xz}$, $D_{yx}$, $D_{yy}$, $D_{yz}$, $D_{zx}$, $D_{zy}$, and $D_{zz}$ are components of the hydrodynamic dispersion coefficient, evaluated at the cell interfaces;

$\mathrm{T}_x$, $\mathrm{T}_y$, and $\mathrm{T}_z$ are cell interface weighting factors used to compute the concentration value at the cell interface from values at the two neighboring nodal points in their repective directions.

If the gird spacing of two neighboring cells is the same along any direction, the weighting factor in that direction is equal to 0.5. The general formulas for the cell interface weighting factors are listed below:

$$\begin{cases} \omega_{x_{j+1/2}} = \dfrac{\Delta x_{j+1}}{\Delta x_j + \Delta x_{j+1}} \\[2ex] \omega_{y_{i+1/2}} = \dfrac{\Delta y_{j+1}}{\Delta y_j + \Delta y_{j+1}} \\[2ex] \omega_{k+1/2} = \dfrac{\Delta z_{k+1}}{\Delta z_k + \Delta z_{k+1}} \end{cases}$$

The components of the dispersion coefficient are calculated from the velocity components and the dispersivities according to equations given in Section 2.3. For example, the values of $D_{xx}$, $D_{xy}$ and $D_{xz}$ are evaluated at the cell interfaces between (i,j,k) and i, j+1,k) along the x direction. The x-component of the Darcy velocity is known directly from the flow model. The y- and z-components are interpolated from Darcy velocities at the interfaces along the y- and z-directions ( see Fig. 4.13):

$$v_{x_{i,j+1/2,k}} = \frac{q_{y_{i,j+1/2,k}}}{\theta_{i,j+1/2,k}} \tag{4.27a}$$

$$v_{y_{i,j+1/2,k}} = \frac{0.5}{\theta_{i,j+1/2,k}} \left[ \left( q_{y_{i-1/2,j,k}} + q_{y_{i+1/2,j,k}} \right) \omega_{x_{j+1/2}} + \left( q_{y_{i-1/2,j+1,k}} + q_{y_{i+1/2,j+1,k}} \right) \left( 1 - \omega_{x_{j-1/2}} \right) \right] \tag{4.27b}$$

$$v_{z_{i,j+1/2,k}} = \frac{0.5}{\theta_{i,j+1/2,k}} \left[ \left( q_{z_{i,j,k-1/2}} + q_{z_{i,j,k+1/2}} \right) \omega_{x_{j+1/2}} + \left( q_{z_{i,j+1,k-1/2}} + q_{z_{i,j+1,k+1/2}} \right) \left( 1 - \omega_{x_{j+1/2}} \right) \right] \tag{4.27c}$$

$$v_{i,j+1/2,k} = \left( v^2_{x_{i,j+1/2,k}} + v^2_{y_{i,j+1/2,k}} + v^2_{z_{i,j+1/2,k}} \right)^{1/2} \tag{4.27d}$$

where $\theta_{i,j+1/2,k} = \omega_{x_{j+1/2}} \theta_{i,j,k} + (1 - \omega_{x_{j+1/2}}) \theta_{i,j+1,k}$ is the porosity at the interface between cell*( i, j, k)* and *(i, j + 1, k).*

The longitudinal and transverse dispersivities are entered into the model on a cell-by-cell basis. Their values at the cell interfaces are interpolated accordingly using the cell weighting factors:

$$\alpha_{L_{i,j+1/2,k}} = \alpha_{L_{i,j,k}} \omega_{x_{j+1/2}} + \alpha_{L_{i,j+1,k}} (1 - \omega_{x_{j+1/2}}) \tag{4.27e}$$

$$\alpha_{TH_{i,j+1/2,k}} = \alpha_{TH_{i,j,k}} \omega_{x_{j+1/2}} + \alpha_{TH_{i,j+1,k}} (1 - \omega_{x_{j+1/2}}) \tag{4.27f}$$

$$\alpha_{TV_{i,j+1/2,k}} = \alpha_{TV_{i,j,k}} \omega_{x_{j+1/2}} + \alpha_{TV_{i,j+1,k}} (1 - \omega_{x_{j+1/2}}) \tag{4.27g}$$

The values of $D_{xx}$ $D_{xy}$ and $D_{xz}$ at the cell interface (*i*, *j* + *1 / 2*, *k*) can be computed as:

$$\begin{aligned} D_{xx_{i,j+1/2,k}} = {} & \alpha_{L_{i,j+1/2,k}} v^2_{x_{i,j+1/2,k}} / v_{i,j+1/2,k} + \alpha_{TH_{i,j+1/2,k}} v^2_{x_{i,j+1/2,k}} / v_{i,j+1/2,k} \\ & + \alpha_{TV_{i,j+1/2,k}} v^2_{x_{i,j+1/2,k}} / v_{i,j+1/2,k} + D_{m_{i,j+1/2,k}} \end{aligned} \tag{4.27h}$$

$$D_{xy_{i,j+1/2,k}} = ( \alpha_{L_{i,j+1/2,k}} - \alpha_{TH_{i,j+1/2,k}}) v_{x_{i,j+1/2,k}} v_{y_{i,j+1/2,k}} / v_{i,j+1/2,k} \tag{4.27i}$$

$$D_{xz_{i,j+1/2,k}} = ( \alpha_{L_{i,j+1/2,k}} - \alpha_{TV_{i,j+1/2,k}}) v_{x_{i,j+1/2,k}} v_{z_{i,j+1/2,k}} / v_{i,j+1/2,k} \tag{4.27j}$$

Similarly, the components of $\boldsymbol{D}_{yx}$, $D_{yy}$, and $D_{yz}$, are calculated at the cell interfaces along the y-direction and $D_{zx}$, $D_{zy}$, and $D_{zz}$ at the cell interfaces along the z-direction, using the same procedure as listed from equations 4.27a to 4.27j.

Fig. 4.13. Evaluation of the velocity components at the cell interfaces in the x direction for calculating components of the dispersion coefficients $D_{xx}$, $D_{xy}$, and $D_{xz}$.

Note that equation 4.25 is solved with the explicit method; therefore, there is a certain stability criterion associated with it. That is, the stepsize can not exceed an upper limit in one transport step. According to Peaceman (1977), the stepsize criterion for equation 4.25 may be expressed as follows:

$$\Delta t \leq \frac{0.5\,R}{\left(\dfrac{D_{xx}}{\Delta x^2} + \dfrac{D_{yy}}{\Delta y^2} + \dfrac{D_{zz}}{\Delta z^2}\right)} \tag{4.28}$$

In the MT3D transport model, equation 4.28 is calculated for each active cell and the minimum ) *t* is taken as the maximum allowed stepsize for solving the dispersion term. This criterion is compared with other time stepsize constraints, if any, to determine the appropriate stepsize for use in the simulation. Obviously, if dispersion is not simulated, then the stability criterion associated with dispersion has no effect on the stepsize in the simulation of other transport processes.

## 4.5 EVALUATION OF THE SINK/SOURCE TERM

The concentration change due to fluid sink and/or source mixing alone can be written as (see Section 3. 1):

$$\frac{DC_{SSM}}{Dt} = -\frac{q_s}{R\,\theta}(C - C_s) \tag{4.29}$$

Equation 4.29 is solved with the fully explicit finite-difference scheme, as in the evaluation of the dispersion term, with the following formula:

$$\Delta C^{n+1}_{SSM\,i,j,k} = -\Delta t \frac{q^{n}_{S\,i,j,k}}{R^{n}_{i,j,k}\,\theta_{i,j,k}}\left(C^{\hat{n}}_{i,j,k} - C^{n}_{S\,i,j,k}\right) \tag{4.30}$$

where $\Delta C^{n+1}_{SSM\,i,j,k}$ is the concentration change due to sink/source mixing from old time level (*n*) to new time level (*n + 1*) at sink or source cell *(i, j, k).* With this explicit scheme, $\Delta C^{n+1}_{SSM\,i,j,k}$cannot exceed the difference between the aquifer concentration $C^{\hat{n}}_{i,j,k}$ , and sink/source concentration, $C^{n}_{S\,i,j,k}$ that is,

$$\frac{\Delta C^{n+1}_{SSM\,i,j,k}}{C^{\hat{n}}_{i,j,k} - C^{n}_{S\,i,j,k}} \leq 1, \qquad C^{\hat{n}}_{i,j,k} \neq C^{n}_{S\,i,j,k} \tag{4.31}$$

or

$$\Delta t \leq \left| \frac{R^{n}_{i,j,k}\ \theta_{i,j,k}}{q^{n}_{S\ i,j,k}} \right| \tag{4.32}$$

where $q^{n}_{S\ i,j,k}$ is the flux of the sink or source per unit volume.

## 4.6 EVALUATION OF THE CHEMICAL REACTION TERM

Chemical reactions currently supported by the MT3D transport model include equilibrium-controlled sorption reactions and first-order irreversible rate reactions, such as radioactive decay or biodegradation.

Sorption is implemented in the model program through use of the retardation factor (*R*). The retardation factor is incorporated into the transport equation in such a way that it becomes a basic parameter in transport simulations. If the sorption isotherms are not simulated in the model, the retardation factor is set to the default value of 1.

If the sorption isotherms are to be simulated, the user must specify the type of sorption isotherm and must input two general sorption equilibrium constants, $S_1$ and $S_2$.

For the linear isotherms the retardation factor is calculated as:

$$R_{i,j,k} = 1 + \frac{\rho_b}{\theta_{i,j,k}} S_1 \tag{4.33}$$

where $D_b$, is bulk density of the porous medium, and $S_1$ represents the distribution coefficient $K_d$ ($S_2$ is not used). Since the retardation factor for linear sorption is independent of the concentration field, it is calculated only once in the beginning of the simulation. Its values remain unchanged throughout the simulation.

For the Freundlich isotherm, the retardation factor is calculated as:

$$R^{n}_{i,j,k} = 1 + \frac{\rho_b}{\theta_{i,j,k}} S_1 S_2 C^{n\ (S_2 - 1)}_{i,j,k} \tag{4.34}$$

where $S_1$ represents the Freundlich constant $K_f$ and $S_2$ represents the Freundlich exponent (see Section 2.5). The Freundlich isotherm is non-linear depending on the concentration field. Therefore, the retardation factor for Freundlich sorption is updated at the beginning of each transport step.

For the Langmuir isotherm, the retardation factor is calculated as:

$$R_{i,j,k} = 1 + \frac{\rho_b}{\theta_{i,j,k}} \left[ \frac{S_1 S_2}{(1 + S_1 C^{\hat{n}}_{i,j,k})^2} \right] \tag{4.35}$$

where $S_1$ represents the Langmuir constant $K_l$ and $S_2$ represents the total concentration of sorption sites available (see Section 2.5). The values of the retardation factor are updated at the beginning of each transport step as the concentration changes.

The concentration change due to the first-order irreversible rate reactions alone can be expressed as:

$$\frac{DC_{RCT}}{Dt} = -\frac{1}{R}(\lambda_1 C + \lambda_2 \frac{\rho_b}{\theta} \overline{C}) \tag{4.36}$$

which reflects the loss of both solute and sorbed mass, or masses gained if the sign of the rate constants, $8_1$ and $8_2$ is negative for simulation of first-order production.

Equation 4.36 is solved using the fully explicit finite-difference scheme as in the evaluation of the dispersion, and sink/source terms:

$$\Delta C^{n+1}_{RCT\,i,j,k} = -\frac{\Delta t}{R^{n}_{i,j,k}} \left( \lambda_1 C^{\hat{n}}_{i,j,k} + \lambda_2 \frac{\rho_b}{\theta_{i,j,k}} \overline{C}^{\hat{n}}_{i,j,k} \right) \tag{4.37}$$

where $\Delta C_{RCT\,i,j,k}^{n+1}$ is the concentration change due to the chemical reaction from old time level (n) to new time level ($n$ + 1) at cell *(i, j, k);* and $\overline{C}_{i,j,k}^{\hat{n}}$ is the sorbed concentration in equilibrium with solute concentration $\overline{C}_{i,j,k}^{\hat{n}}$ in the same cell:

$$\left\{\begin{array}{ll} \overline{C}_{i,j,k}^{\hat{n}} = S_1\, C_{i,j,k}^{\hat{n}}\ , & \textit{for Linear isotherm}\ ; \\ \overline{C}_{i,j,k}^{\hat{n}} = S_1\, C_{i,j,k}^{\hat{n}\ (S_2-1)}\ , & \textit{for Freundlich isotherm}\ ; \\ \overline{C}_{i,j,k}^{\hat{n}} = \dfrac{S_1 S_2\, C_{i,j,k}^{\hat{n}}}{1 + S_1 C_{i,j,k}^{\hat{n}}}\ , & \textit{for Langmuir isotherm}\ . \end{array}\right. \qquad (4.38)$$

The stability criterion associated with this explicit scheme is,

$$\Delta t \leq \min\left(\frac{1}{|\lambda_1|}, \frac{1}{|\lambda_2|}\right) \qquad (4.39)$$

## 4.7 MASS BUDGET

A mass budget is calculated at the end of each transport step and accumulated to provide summarized information on the total mass into or out of the groundwater flow system. The discrepancy between the total mass in and out also serves as an indicator of the accuracy of the simulation results.

Sources that release mass into the aquifer system, and sinks that remove mass from the aquifer system, include constant-concentration boundaries, constant-head boundaries, generalhead-dependent boundaries, wells, drains, rivers, recharge, evapotranspiration and chemical reactions. In addition, mass release from aquifer storage and mass accumulation in aquifer storage are also considered as sources and sinks inasmuch as release from mass storage effectively adds mass to the groundwater flow system and accumulation in mass storage effectively removes mass from the groundwater flow system. The difference is that the changes in mass storage do not involve mass entering or leaving the aquifer as with other types of sources or sinks. The mass accumulated in or released from mass storage includes the solution phase (solute mass) and the solid phase (sorbed mass) if sorption is simulated.

The difference between the total mass in and out is calculated, as a percent error, using the following formula:

$$ERROR = \frac{100\ (IN - OUT\ )}{(IN + OUT\ )/2} \tag{4.40}$$

where *IN* is total mass into the groundwater flow system from external sources plus mass release from storage as a result of the decrease in solute and sorbed concentrations; and *OUT* is total mass out of the groundwater flow system through sinks plus mass accumulation in storage as a result of the increase in solute and sorbed concentrations. *ERROR* is the percentage discrepancy between *IN* and *OUT*. Generally, the mass balance error is an indication of the validity of a numerical solution and it should be small for the numerical solution to be acceptable.

Unlike the pure finite-difference method, the mixed Eulerian-Lagrangian schemes presented in the preceding discussions are not entirely based on the principle of mass conservation. In other words, due to the discrete nature of moving particles, the solution to the transport equation does not guarantee that the mass into a cell will equal the mass out of that cell in a particular transport step. This can be best illustrated in the following example. Assume that a well as shown in Fig. 4.14 is continuously injecting water of a certain concentration at a fixed rate into Cell 1, which has the same concentration as the injected water. All cells except Cell 1 have zero initial concentration. Suppose that 4 moving particles are placed at Cell 1. It is obvious that it takes some time before the particles move into Cell 2. Until that time (denoted as $t_o$), there is no change in the aquifer mass storage, but there is flow of mass into the aquifer from the injection well. Therefore, if the transport stepsize selected for the simulation is smaller than $t_o$, the mass balance discrepancy is 200 percent for the first step because the *OUT* term is equal to 0 while the *IN* term is not. This, of course, does not mean the solution is incorrect; it is simply a characteristic of moving particle methods and of the selection of the stepsizes. As the simulation goes on, the mass balance error should decrease to near zero as the increase in mass storage due to the increase in aquifer concentrations approximates the mass entering the aquifer from the injection well. Therefore, is generally not very meaningful to look at the

Fig. 4.14. Example of mass balance discrepancy due to discrete nature of moving particle methods.

mass balance at a particular step with moving particle methods; rather, it is the averaged and accumulated mass balance information that is more indicative of the overall acceptability of the simulation.

The mixed Eulerian-Lagrangian solution schemes implemented in the MT3D transport model provides many options which can be adjusted to achieve minimal mass balance discrepancy. These options include the number and initial distribution pattern of moving particles, different particle tracking schemes, and the selection of optimal stepsizes.

## 4.8 A Note on the Pure Finite-Difference Method

The pure finite-difference method solves all terms in the transport equation using the finite-difference scheme. The word "pure" is used to distinguish it from the mixed Eulerian-Lagrangian method utilized in the MT3D transport model which solves the advection term using one of the method-of-characteristics schemes and the other terms using the finite-difference scheme. The pure finite-difference method can lead to significant numerical dispersion for problems having very sharp concentration fronts. However, because the pure finite-difference method does not involve any particle tracking calculation or concentration interpolation, it is normally more efficient computationally. Furthermore, because the finite-difference method is entirely based on the principle of mass conservation, it should have very small mass balance discrepancy at every step. For these reasons, a finite-difference routine has also been provided in the MT3D model to supplement the MOC, MMOC or HMOC scheme for solving the advection term.

The finite-difference routine solves the unexpanded advection term and the sink/source directly based on an upstream weighting scheme as given below:

$$
\begin{aligned}
\frac{\partial}{\partial x_i}(v_i C) = {} & \frac{v_{x\ i,j+1/2,k}\, C_{i,j+1/2,k} - v_{x\ i,j-1/2,k}\, C_{i,j-1/2,k}}{\Delta x_j} \\
& + \frac{v_{y\ i+1/2,j,k}\, C_{i+1/2,j,k} - v_{x\ i-1/2,j,k}\, C_{i-1/2,j,k}}{\Delta y_i} \\
& + \frac{v_{z\ i,j,k+1/2}\, C_{i,j,k+1/2} - v_{z\ i,j,k-1/2}\, C_{i,j,k-1/2}}{\Delta z_k}
\end{aligned}
\qquad (4.41)
$$

where

$$C_{i,j+1/2,k} = \begin{cases} C_{i,j,k}, & \text{if } v_{x\ i,j+1/2,k} \succ 0 \\ C_{i,j+1,k}, & \text{if } v_{x\ i,j+1/2,k} \prec 0 \end{cases}$$

$$C_{i+1/2,j,k} = \begin{cases} C_{i,j,k}, & \text{if } v_{y\ i+1/2,j,k} \succ 0 \\ C_{i+1,j,k}, & \text{if } v_{y\ i+1/2,j,k} \prec 0 \end{cases}$$

$$C_{i,j,k+1/2} = \begin{cases} C_{i,j,k}, & \text{if } v_{z\ i,j,k+1/2} \succ 0 \\ C_{i,j,k+1}, & \text{if } v_{z\ i,j,k+1/2} \prec 0 \end{cases}$$

# Chapter 5
# PROGRAM STRUCTURE AND DESIGN

## 5.1 OVERALL STRUCTURE

The computer program of the MT3D transport model uses a modular structure similar to that implemented in the U. S. Geological Survey modular three-dimensional finite-difference groundwater flow model, or MODFLOW, (McDonald and Harbaugh, 1988). Like the MODFLOW model, the MT3D model consists of a main program and a large number of highly independent subroutines, called modules, which are grouped into a series of "packages". Each of these packages deals with a single aspect of the transport simulation. The similarity between MT3D and MODFLOW in the program structure and design is intended to facilitate the use of the MT3D transport model in conjunction with MODFLOW, one of the more widely used flow models.

The general procedures performed in the transport model for a typical simulation run are illustrated in Fig. 5.1. The simulation time is divided into "stress periods", also referred to as "pumping periods", within which the stress (i.e., the sink/source) parameters are constant. Each stress period, in turn, is divided into a series of time steps. The hydraulic heads and fluxes at each time step are solved by the flow model and used by the transport model. Since the flow equation is generally solved using an implicit interactive method whereas the transport equation is solved in the MT3D model with an explicit direct method, the length of each time step for the head solution may exceed the limitation required for stability in the transport solution. Thus, each time step used in obtaining the head solution is further divided into a number of smaller time increments, termed transport steps, within which the hydraulic heads and fluxes are assumed to be constant.

Fig. 5.1. General procedures for a typical transport simulation.

Prior to entering the stress period loop, the program executes three procedures which pertain to the simulation as a whole (see Fig.5.1). In the Define procedure, the simulation problem is defined; that is, the size of the model, the number of stress periods, and the various transport options to be used in the simulation are specified. In the Allocate procedure, computer memory is allocated for the data arrays whose dimensions depend on the parameters specified in the Define procedure. In the Read & Prepare procedure, input data that are constant throughout the simulation are read and processed. These input data include spatial and temporal discretization information, boundary conditions, initial conditions, transport parameters, solution parameters, and output control options.

The first procedure within the stress period loop is the Stress procedure which obtains timing information for the current stress period: the length of the stress period, the number of time steps within the stress period, and the length of each time step. A second Read & Prepare procedure then reads and prepares input data which are constant within the current stress period, i.e., the concentrations of those sources or sinks that need to be specified. The transport model obtains the location, type, and flow rates of all sources and sinks simulated in the flow model from an unformatted head and flow file saved by the flow model. Source concentrations are automatically set equal to zero unless the user specifies a different concentration through this Read & Prepare procedure. Sink concentrations are always set equal to the concentration in the aquifer at the sink location, except for evapotranspiration, whose concentration can be specified through this Read & Prepare procedure.

Within the time step loop, A third Read & Prepare procedure reads and processes the hydraulic heads and flow terms saved by the flow model, automatically incorporating the specified hydrologic boundary conditions. The Coefficient procedure then calculates certain coefficients that are constant within each time step of the head solution, such as the dispersion coefficient.

The transport step loop contains four procedures. The Advance procedure determines an appropriate stepsize for use in the current transport step. The Solve procedure solves each transport component with an explicit mixed Eulerian-Lagrangian solution scheme and calculates the mass into or out of the aquifer through each component. The Budget procedure calculates and prepares global mass balance information; and the Output procedure prints or saves simulation results as needed according to the user-specified output control options.

The general procedures outlined in the preceding discussion are implemented for each of the four components in the transport equation: advection, dispersion, sink/source mixing, and chemical reactions. The implementation is done through the use of individual modules, or highly independent subroutines, each of which performs one particular procedure. For example, the advection component is implemented through 3 modules, named ADV1AL, ADV1RP, and ADV1SV, respectively, where ADV indicates the transport component (advection) for which these modules are implemented. The number (1) indicates the current version number of the computer code. AL (abbreviation for Allocate) , RP (abbreviation for Read & Prepare), and SV (abbreviation for Solve) indicate the procedures these modules perform. These modules, which are called by the main program, are termed primary modules to distinguish them from secondary modules, which are used only inside the primary modules to which they belong. The primary modules ADV1AL, ADV1RP, and ADV1SV and their associated secondary modules are grouped into a "package", called the Advection Package (abbreviated as ADV) (see Fig. 5.2). Dispersion, sink/source mixing, and chemical reactions are similarly implemented and grouped into the Dispersion Package (DSP), Sink & Source Mixing Package (SSM), and Chemical Reaction Package (RC7).

In addition to the four transport component packages, the MT3D model program includes three additional packages: the Basic Transport Package (BTN), the Flow Model Interface Package (FMI), and the Utility Package (UTL). The Basic Transport Package handles basic tasks that are required by the transport model as a whole.  Among these tasks are definition of the simulation problem, specification of the initial and boundary conditions, determination of appropriate transport stepsize, preparation of global mass balance information and output of simulation results.  The Flow Model Interface Package interfaces with a flow model to obtain the flow solution from the flow model.  Currently, the interfacing is done through an unformatted disk file, containing hydraulic heads and various flow and sink/source terms solved by the flow model.  This file is read and processed in the form needed by the transport model.  The Utility Package contains several utility modules which are called upon by other modules to perform general computer input and output tasks.

All of the the primary modules contained in the MT3D transport model as organized by package and procedure are shown in Fig. 5.2. All the packages documented in this report are listed in Table 5. 1. Note that there is no independent solver package included because the current version of the MT3D transport model uses explicit solution schemes.  Therefore, each component of the transport equation is solved directly wiithin its respective package.

Fig. 5.2. Primary modules of MT3D as organized by procedures and packages.

**Table 5.1. List of packages included in the MT3D transport model.**

| Package Name | Abbreviation | Package Description |
|---|---|---|
| Basic<br>entire  Transport | BTN | Handles basic tasks that are required by the transport model . Among these tasks are definition of the problem, specification of the boundary and initial conditions, determination of the stepsize, preparation of mass balance information, and printout of the simulation results. |
| Flow Model | FMI | Interfaces with a flow model. Currently, the interfacing is done through an unformatted disk file containing heads and flow terms. The FMI Package reads the contents of this file and prepares heads and flow terms in the form needed by the transport model. |
| Advection | ADV | Solves the concentration change due to advection with one of the three mixed Eulerian-Lagrangian schemes included in the package: MOC, MMOC,  or HMOC. |

| | | |
|---|---|---|
| Dispersion | DSP | Solves the concentration change due to dispersion with the explicit finite difference method. |
| Sink & Source Mixing | SSM | Solves the concentration change due to fluid sink/source mixing with the explicit finite difference method. Sink/source terms may include wells, drains, rivers, recharge and evapotranspiration. The constant-head boundary and general-head-dependent boundary are also handled as sink/source terms in the transport model. |
| Chemical chemical Reactions | RCT | Solves the concentration change due to reactions. Currently, the chemical reactions include linear or nonlinear sorption isotherms and first-order irreversible rate reactions (radioactive decay or biodegradation). |
| Utility | UTL | Contains a number of utility modules that are called upon by primary modules to perform such general-purposed tasks as input/output of data arrays. |

## 5.2 MEMORY ALLOCATION

The main computer memory required to run the MT3D model is allocated at program execution time in two one-dimensional storage arrays called the "X" array for real variables and the "IX" array for integer variables. The real X and integer IX arrays are then partitioned to store individual date arrays whose dimensions depend on the problems to be simulated. The sizes of individual arrays are calculated and accumulated by the Allocate procedure of their respective packages; the accumulated sizes serve as pointers indicating the locations of individual arrays within the X or IX array. If the accumulated sizes of the individual arrays exceed the length of the X or IX array which is preset at program compilation, program execution stops. If this happens, the length of the X or IX array must be increased by modifying the following parameter statement in the main program:

```
PARAMETER (LENX=450000, LENIX=36000)
```

where `LENX` is the length of the X array and `LENIX` the length of the IX array. The lengths of the X and IX arrays required for a specific problem depend on the type and number of packages used. The length of the X array will generally range from 10 to 30 times the number of cells in the grid plus 4 times the maximum number of moving particles allowed; the length for the IX array is approximately 2 to 4 times the number of cells. The exact sizes of the X and IX arrays can be calculated according to the instructions in Appendix A. They can also be known by simply running the program, which will print out the required X and IX sizes before it stops execution if either one or both of these arrays are dimensioned too small.

The MT3D model program is written for three-dimensional simulation. When the program is used for one- or two-dimensional applications, some arrays are not needed and to save memory storage, these arrays are not allocated space in the X or IX array. For example, array QZ is intended for storing fluxes between vertical layers. If the program is used to simulate a two-dimensional problem in plan view, QZ is not needed and thus is not allocated storage space; and as a result, it is never used, or operated upon, in any way in the program. This is important to keep in mind when the user wants to modify the computer code.

## 5.3 INPUT STRUCTURE

The input structure of the model program is designed to gather input data from as many different files as needed in a simulation. This structure is similar in many ways to that of MODFLOW. Therefore, the users who are familiar with MODFLOW should find it very easy and straightforward to prepare input for the MT3D model.

The Basic Transport Package is always used in every simulation. Thus, an input file for the Basic Transport Package is required every time the program is run. In the input file to the Basic Transport Package, there is a record containing the logical TRNOP array. Each element of the TRNOP array corresponds to a major option, generally a package (see Fig. 5.3). An option is invoked by setting the value of its corresponding TRNOP element to T (for True), and turned off by setting the value to F (for False). When an option is used, an input file containing data exclusively for that option is then required. For example, the second element of the TRNOP array corresponds to the Dispersion Option (or Package). If it is necessary to simulate dispersion, the second TRNOP array element must be entered as T. An input file containing dispersion parameters must be created and read by the program.

In addition to the main input file for the Basic Transport Package and the input files for the various transport component packages which are used, the transport model always requires another input file which contains hydraulic heads, fluxes across cell interfaces, and the location and flow rate of sinks and/or sources. This file is generated by a flow model used in conjunction with the transport model, and read by the Flow Model Interface Package of the MT3D model. The structure and form of this file are discussed in Chapter 6.

In the standard ANSI FORTRAN 77 language, a data file must be opened with a FORTRAN unit number and a file name before it can be accessed by the program. This is done in the subroutine OPENFL which is included in the Utility Package. The file names can be entered interactively from the monitor screen or through a response file in a batch mode as discussed in the next chapter. The unit numbers associated with major input files are preset in the main program. They can be changed, if necessary, by modifying the following parameter statement in the main program:

```
PARAMETER (INBTN=l,INADV=2,INDSP=3,INSSM=4,INRCT=9,INUHF=10)
```

where

`INBTN` is the unit number for the Basic Transport Package;

`INADV` is the unit number for the Advection Package;

`INDSP` is the unit number for the Dispersion Package;

`INSSM` is the unit number for the Sink & Source Mixing Package;

`INRCT` is the unit number for the Chemical Reaction Package; and

`INUHF` is the unit number for the unformatted head & flow file, read by the Flow Model Interface Package.

Once the unit number associated with a package is used in the simulation, it must not be used again elsewhere.

## 5.4 OUTPUT STRUCTURE

The program generates a standard output file and several optional output files. The standard output file is generated every time the model is run. The optional output files are generated only if they are requested. The amount, type, and frequency of information to be written on the output files are controlled by the user-specified options in the input file to the Basic Transport Package. The functions of these output files are listed below:

1. The Standard Output File: contains echo of input data to ensure they are read in properly, printout of simulated concentrations, and some other essential information such as model-calculated parameters and mass budget at user-specified times and at the end of the simulation.

2 . The Unformatted Concentration File (default name: MT3D.UCN): contains concentrations saved at user-selected times in the unformatted form for a continuation run or for post-processing purposes.

3. The Observation Point File (default name: NMD.OBS): contains concentrations versus total elapsed time at user-specified observation points at every transport step.

4. The Mass Balance Summary File (default name: MT3D.MAS): contains a one-line summary of mass budget at every transport step for checking purposes.

5. The Model Grid Configuration File (default name: MT3D.CNF): contains model spatial discretization information to be used by the post-processor for graphic presentation.

The unit numbers associated with these output files are preset in the following parameter statement in the main program:

```
PARAMETER (IOUT=ll, IUCN=12, IOBS=13, IMAS=14, IUCN=15)
```

where

`IOUT` istheunitnumberfortheStandardOutputFile;

`IUCN` is the unit number for the Unfonnatted Concentration File, MT3D.UCN;

`IOBS` is the unit number for the Observation Point File, MT3D.OBS;

`IMAS` is the unit number for the Mass Balance Summary File, MT3D.MAS;

`ICNF` is the unit number for the Model Grid Configuration File, MT3D.CNF.

These unit numbers can be changed, ff necessary, by modifying the above parameter statement.

## 5.5 COMPUTER PROGRAM DESCRIPTION

The computer program of the MT3D transport model is written in the standard FORTRAN 77 language as defined by the American National Standards Institute (ANSI). To maximize the portability of the computer program, only language features pertaining to the ANSI standard are used except the `IMPLICIT NONE` statement. The use of this statement requires the explicit declaration of all variables' types and is extremely helpful in preventing variable names from being misspelled, a common error in writing or modifying programs. If the compiler the user has does not support this extension, the `IMPLICIT NONE` statement in all subroutines should be commented out. Furthermore, all real variables in the program are declared as single precision. If it is necessary to run the model in double precision, modify all statements starting with `REAL * 4` in each subroutine to `REAL * 8.`

The main program and all subroutines of the MT3D program (including primary and secondary modules) are described briefly in the following sections. For more information, the user may refer to the extensively commented source code included in the disk and listed in Appendix F.

### 5.5.1 Main Program -- *MTMAIN*

The main program controls the overall execution of the entire program. A flow chart showing all the primary modules called by the main program is provided in Fig. 5.4. The basic steps of the main program for each simulation are:

1. Set the lengths of the X and DC arrays.

2. Assign unit numbers to major input and output files and open these files.

3. Define the simulation problem in terms of layers, rows, columns, stress periods, and major transport options to be used.

4. Allocate space in the X and IX arrays for all individual data arrays.

5 . If either X or IX array is not dimensioned large enough, stop.

6 . Read and process input data which are constant throughout the simulation.

7 . For each stress period:

    (a) Obtain stress period timing information.

    (b) Read and process the concentrations of sources or sinks that need to be specified.

    (c) For each time step:

        (1) Read hydraulic heads, fluxes across cell interfaces, and the locations and flow rates of sinks or sources.

        (2) Calculate coefficients that are constant within the current dm step.

        (3) For each transport step:

            (i) Determine an appropriate stepsize for the current transport step.

            (ii) Solve each component of the transport equation.

            (iii) Prepare mass balance information.

            (iv) Print or save simulation results.

            (v) If the number of transport steps exceeds the specified maximum, stop.

8. End program.

Fig. 5.4. Flow chart for the main program showing all modules.

### 5.5.2 Basic Transport Package -- *MTBTNI*

The Basic Transport Package consists of eight primary modules, each of which is described below in the order of execution:

BTNLDF Define the simulation problem by reading the number of layers, rows, columns and stress periods as well as the transport options to be used;
BTNLAL Allocate space for basic data arrays needed by the model as a whole;
BTNLRP Read and prepare basic data arrays used by the entire model;
BTNLST Read stress period timing information;
BTNLAD Determine an appropriate stepsize for each transport step;
BTNLSV Update cell concentrations and prepare for simulation of the next step;
BTNLBD Prepare global mass balance information;
BTN10T Print or save simulation results according to the user-specified options.

### 5.5.3 Flow Model Interface Package -- *MTFMI]*

The Flow Model Interface Package consists of two primary modules and three secondary modules:

FM11RP1 Read and prepare hydraulic heads and fluxes across cell interfaces in the column, row and layer directions on a cell-by-cell basis by calling secondary module READHQ.
FM11RP2 Read and prepare the locations and flow rates of the various sink/source terms by calling secondary modules READPS (for reading point sinks or sources) and READDS (for reading areally distributed sinks or sources).

### 5.5.4 Advection Package -- *MTADVI*

The Advection Package consists of three primary modules and a number of secondary modules:

ADVLAL Allocate space for data arrays needed by the Advection Package;
ADVLRP Read and prepare input data needed for solving the advection term;
ADVISV Solve the advection term. This primary module includes the following secondary modules, which are named according to the function they perform:

*LOCATE:* Find cell indices (J,I,K) of a particle located at coordinates (x,y,z);
*VPOINT:* Interpolate particle velocity at an arbitrary point based on the piecewise linear scheme;
*EULER:* Perform particle tracking with the first-order Euler algorithm;
*RK4:* Perform particle tracking with the fourth-order Runge-Kutta algorithm;

*PARMGR:* Manage the distribution of moving particles dynamically, inserting or deleting particles as necessary;
*CNGRAD:* Calculate relative concentration gradient of a cell with its neighboring cells;
*GENPTN:* Insert particles in a finite-difference cell according to fixed
patterns;
*GENPTR:* Insert particles in a finite-difference cell randomly;
*CPOINT.* Calculate concentration at an arbitrary point from neighboring nodes with the first-order polynomial interpolation;
*QCFLUX* Compute mass flux into or out of a finite-difference cell based on finite-difference formulation.

### 5.5.5 Dispersion Package -- *MTDSPI*

The Dispersion Package consists of four primary modules, each of which is described below in the order of execution:

DSPLAL Allocate space for data arrays needed by the Dispersion Package;
DSPLRP Read and prepare dispersion parameters;
DSPLCF Calculate components of the hydrodynamic dispersion coefficient;
DSPI SV Solve the dispersion term using the explicit finite difference formulation;

### 5.5.6 Sink & Source Mixing Package -- *MTSSMI*

The Sink & Source Mixing Package consists of three primary modules, each of which is described below in the order of execution:

SSM1AL Allocate space for data arrays needed by the Sink & Source Mixing Package;
SSM1RP Read and prepare concentrations of sources and/or sinks that need to be specified;
SSM1SV Solve the concentration change due to sink/source mixing using the explicit finite difference formulation.

### 5.5.7 Chemical Reaction Package -- *MTRCTI*

The Chemical Reaction Package consists of three primary modules and a secondary module:

RCT1AL  Allocate space for data arrays needed by the Chemical Reaction Package;
RCT1RP  Read and prepare chemical reaction parameters;
RCT1SV  Solve the concentration change due to chemical reactions using the explicit finite difference formulation.
Both RCTLRP and RCTLSV use the following secondary module:
*RFCOEF:* Calculate retardation factor for linear or non-linear sorption isotherms.

### 5.5.8 Utility Package -- *MTUTLI*

The Utility Package consists of the following utility subroutines called upon by other modules to perform general computer input/output tasks:

OPENFL  Open an input or output file;
RARRAY  Read a one- or two-dimensional REAL data array using the block, zonal, list-directed, unformatted, or any user-specified format;
IARRAY  Read a one- or two-dimensional INTEGER data array with the block, zonal, list-directed, unformatted, or any user-specified format;
RPRINT  Print a one- or two-dimensional REAL data array with the wrap or strip format;
IPRINT  Print a one- or two-dimensional INTEGER data array with the wrap or strip format.

# Chapter 6
# INPUT INSTRUCTIONS

## 6.1 GENERAL INFORMATION

The MT3D model program uses a combination of formatted, list-directed and unformatted input forms, and calls two general array readers to enter data arrays. These input forms and the array readers are described in this section for easy reference in the preparation of input files.

### 6.1.1 Input Forms

Formatted

If an input value is entered using the formatted form, the type of value and the space it occupies must agree with its format specifier. Four types of input variables are used in the program: Integer, Real, Character and Logical.

In the input instructions to be followed, the format specifier for integer variables is written as `Iw` where `I` implies that the variable must have the form of an integer (it must not contain a decimal point or exponent); and `w` is the number of spaces reserved for the variable. If the input value is less than `w` spaces wide, the unoccupied spaces are treated as blanks by default. It is always good practice to enter the value right-justified.

The format specifier for real variables is written as `Fw.d` where `w` is the number of spaces reserved for the entire input value, with the fractional part taking `d` spaces. When a decimal point is present, it overrides the `d` specified in the format. Thus, even though the specifier for real variables is written as `F10.0` in the input instructions, input values can be entered in such forms as `12.345` or `0.12345`. Furthermore, input values in the exponential form, such as `1.2345E-5`, are also acceptable.

The format specifier for the character variable is written as `Aw` where `w` is the number of spaces reserved for the character variable. If the character string is less than `w` characters wide, unfilled spaces are treated as blanks.

Finally, the format specifier for the logical variables is written as `Lw` where w is the number of spaces reserved for the logical variable. The logical variable must be entered either as `T` (for True) or as `F` (for False), leaving unoccupied spaces blank.

List-Directed

List-directed input (also referred to as free format) has several characteristics: (1) a list-directed record is a sequence of values separated by either commas or blanks with multiple blanks allowed; (2) a list-directed record terminates when the number of the input values equals the number of items in the input list or until a slash (/) is encountered; (3) a list-directed record may occupy several lines of an input file, but each new record should start at a new line; and finally, (4) list-directed input permits the use of a repeat count in the form,

$n*d$

where n is an unsigned-nonzero integer constant, and the input $n*d$ causes n consecutive values of d to be entered.

Unformatted

An unformatted file is a sequence of unformatted records in the form of binary characters. An unformatted file cannot be visually examined, but is smaller in size and faster to process than a formatted file. The model program uses the unformatted form to enter the hydraulic heads and flow terms saved by a flow model.

### 6.1.2 Array Readers RARRAY and IARRAY

Most of the input data to be entered to the model by the user will consist of one- or two-dimensional real or integer arrays. Three-dimensional arrays are treated as a series of two-dimensional arrays, each of which corresponds to an individual model layer and is entered in sequence according to the layer number.

In the MT3D model, arrays are entered as an "array-control record", plus, optionally, a series of records containing the array elements. If all the elements of an array have the same value, the value is specified on the control record and it is not necessary to read the associated array. If the array elements vary, records containing the array values are read using the various input forms as specified on the array-control record. To perform these tasks, two utility subroutines, RARRAY for reading one- or two-dimensional real arrays, and IARRAY for reading one- or two-dimensional integer arrays, are provided in the program. These two array readers are compatible to array readers U2DREL and U2DINT provided in the MODFLOW model (McDonald and Harbaugh, 1988). However, RARRAY and IARRAY also permit the input of array values by block, zonal and list-directed (or free) formats.

For each array to be entered, RARRAY or IARRAY reads an array-control record first on the unit reserved for the major option which calls the array reader. For example, unit 1 is preset for the Basic Transport Package, thus, RARRAY or IARRAY reads the array-control record in the input file for the Basic Transport Package from unit 1. The content and form of the array control record are as follows:

FOR REAL ARRAY READER (RARRAY):

| | | | | |
|---|---|---|---|---|
| Record: | IREAD | CNSTNT | FMTIN | IPRN |
| Format: | I10 | F10.0 | A20 | I10 |

FOR INTEGER ARRAY READER (IAARRAY):

| Record: | IREAD | ICONST | FMTIN | IPRN |
|---|---|---|---|---|
| Format: | I10 | I10 | A20 | I10 |

Explanations

IREAD--determines how array values are read.

If IREAD=0, every element in array will be set equal to the value CNSTNT for RARRAY, or ICONST for IARRAY.

If IREAD=100, an array of input values follows the control record. The array values are read in the format specified in the third field of the array-control record (FMTIN), from the same unit used for reading the array-control record (see Fig. 6. 1).

If IREAD=101, an array of values organized in "block" format follows the array-control record. The block format consists of a record specifying the number of blocks, NBLOCK, followed by NBLOCK records of input values (all in free format), specifying the first row (Il), last row (I2), first column (Jl), last column (J2) of each block as well as the value (ZZ/IZ) to be assigned to the cells within the block (ZZ is a real value for RARRAY and IZ is an integer value for IARRAY), as shown below:

| | |
|---|---|
| NBLOCK | (free format) |
| I1, I2, J1, J2, ZZ/IZ (block 1) | (free format) |
| I1, I2, J1, J2, ZZ/IZ (block 2) | (free format) |
| . . . . . . . . | |
| I1, I2, J1, J2, ZZ/IZ (block NBLOCK) | (free format) |

If a subsequent block overlaps any preceding blocks, the subsequent block overrides the preceding blocks. It is always good practice to have the first block cover the entire grid and allow subsequent blocks to override portions of the grid as this averts the possibility that any portion of the grid will be left unassigned (see Fig.6. 1).

If IREAD=102, an array of values organized in "zonal" format follows the array-control record. Each zone represents one value of the input variable, and each zone is identified by a zone number -- an integer which may actually be thought of as a code for the corresponding value of the input variable. The zonal format consists of a record specifying the number of zones, NZONE, followed by an array of values for the input variables, ZV(NZONE) or IZV(NZONE), which are listed in sequence according to zone numbers (1, 2, 3, ..., etc); ZV is a real array for RARRAY and IZV is an integer array for IARRAY as explained below. Following ZV/IZV is the zone indicator array A(NCOL,NROW)/IA(NCOL,NROW) specifying the zone number assigned to each node (cell) in a given layer of the model. The elements in this array are actually always integers, i.e., the integer codes identifying the zone for each cell. However, they are stored in the array reserved for input variable itself, and thus follow the format of the input variable. Hence, the zone indicators are read using the format as specified in the third field of the array-control record (FMTIN) which must be a real format specifier for RARRAY and an integer format specifier for IARRAY. If the zone indicator for a cell is equal to zero, the value for that cell is set to zero (see Fig. 6. 1).

The zonal format for RARRAY:

| | |
|---|---|
| NZONES | (free format) |
| ZV(l),.ZV(2).......... ZV(NZONE) | (free format) |
| A(NCOL,NROW) | (using format FMTIN) |

The zonal format for IARRAY:

| | |
|---|---|
| NZONE | (free format) |
| IZV(l), IZV(2)........ IZV(NZONE) | (free format) |
| IA(NCOL,NROW) | (using format FMTIN) |

If IREAD=103, an array of values follows the array-control record. The array values are read using list-directed or free format (see Fig. 6. 1).

If IREAD=any value other than 0, 100, 101, 102, and 103, array values are read from a separate file.

If IREAD>O, it is the unit number on which the external file is read using the format specified in FMTIN.

If IREAD<O, the absolute value of IREAD gives the unit number on which the array values are read from an external unformatted file. The unformatted file contains one dummy record, followed by an unformatted record of NCOL*NROW values.

CNST'NT/ICONST--is a constant. Its use depends of the value of IREAD.

If IREAD=0,every element in the array is set equal to CNSTNT/ICONST.

If IREAD…0, and CNSTNT/ICONST…0, elements in the array are multiplied by CNSTNT/ICONST.

FMTIN--is the format specifier used to read array values or the zonal indicator array. The format must be enclosed in parentheses; for example, (15F5.0) for real values and (15I5) for integer input values.

IPRN--is a flag indicating whether the array being read should be printed out for checking and also serves as a code indicating the format that should be used in printing. It is used only if IREAD is not equal to zero. IPRN is set to zero if the specified value exceeds those defined in Table 6.1 as shown below. If IPRN is less than zero, the array will not be printed.

Table 6.1. Printing formats corresponding to the EPRN code.

(After McDonald and Harbaugh, 1988)

| IPRN | RARRAY | IARRAY |
|---|---|---|
| 0 | 10G11.4 | 10I11 |
| 1 | 11G10.3 | 60Il |
| 2 | 9G13.6 | 40I2 |
| 3 | l5F7.1 | 30I3 |
| 4 | 15F7.2 | 25I4 |
| *5* | 15F7.3 | 2015 |
| 6 | 15F7.4 | |
| 7 | 20F5.0 | |
| 8 | 20F5.1 | |
| 9 | 20F5.2 | |
| 10 | 20F5.3 | |
| 11 | 20F5.4 | |
| 12 | l0G11.4 | |

```
                 CNSTNT                   FMTIN       IRPN
       IREAD
         100          0.                (l0F5.1)          3
 2.1     2.1    2.1    2.1   2.1   2.1   2.1    2.1   2.1    2.1
 2.1     2.1    2.1    2.1   2.1   2.1   2.1    2.1   2.1    2.1
10.2    10.2   10.2   10.2  10.2  10.2  10.2   10.2  10.2   10.2
10.2    10.2   10.2   10.2  10.2  10.2  10.2   10.2  10.2   10.2
23.5    23.5   23.5   23.5  23.5  23.5  23.5    0.4   0.4    0.4
23.5    23.5   23.5   23.5  23.5  23.5  23.5    0.4   0.4    0.4
23.5    23.5   23.5   23.5  23.5  23.5  23.5    0.4   0.4    0.4
23.5    23.5   23.5   23.5  23.5  23.5  23.5    0.4   0.4    0.4
23.5    23.5   23.5   23.5  23.5  23.5  23.5    0.4   0.4    0.4
   0       0      0      0     0     0     0    0.4   0.4    0.4
```

(a) An array of 10 x 10 is read with the user-specified format (l0F5.1) (IREAD= 100).

```
                101                0.          (FMTIN not used)        3
 5     <-------------           NBLOCK
  1       10        1        10        0
```

```
        1       2       1       10      2.1
        3       4       1       10     10.2
        5       9       1        7     23.5
        5      10       8       10      0.4
```

(b) The same array as shown in (a) is read using the block format (IREAD=101).

```
   102       0.                    (l0F5.0)                  3
4             <--------- NZONE
      2.1   10.2      23.5           0.4        <--------  ZZ(NZONE)
         1       1       1       1       1       1       1       1       1       1
         1       1       1       1       1       1       1       1       1       1
         2       2       2       2       2       2       2       2       2       2
         2       2       2       2       2       2       2       2       2       2
         3       3       3       3       3       3       3       4       4       4
         3       3       3       3       3       3       3       4       4       4
         3       3       3       3       3       3       3       4       4       4
         3       3       3       3       3       3       3       4       4       4
         3       3       3       3       3       3       3       4       4       4
         0       0       0       0       0       0       0       4       4       4
```

(c) The same array as shown in (a) is read using the zonal format (IREAD=102). Note that format (I0F5.0) is used to read the zone indicators).

```
   103                                 0.         (FMTIN not used)              3
20*2.1       20*10.2  7*23.5  3*0.4  7*23.5   3*0.4  7*23.5   3*0.4   7*23.5   3*0.4
7*23.5        3*0.4    7*0     3*0.4
```

(d) The same array as shown in (a) is read using the list-directed format (IREAD=103).

Fig. 6.1. Illustration of the various input forms used by RARRAY and IARRAY.

## 6.2 UNITS OF INPUT AND OUTPUT VARIABLES

The MT3D transport model uses consistent units for input and output variables. In the input file to the Basic Transport Package, the user decides the units for time, length and mass. Then, any input variable or constant should be entered in units consistent with the three basic units. For example, suppose that DAY is chosen as unit for time, FT for length and LB for mass. Then, hydraulic heads should have the unit of FT, solute concentration the unit of LB/FT$^3$ , dispersivity the unit of FT, distribution coefficient for linear sorption the units of FT$^3$ /LB, and so on. If SI units are preferred, and S(ECOND), CM(CENTMETER) and G(RAM) are selected as the units for time, length and mass, respectively, then, heads should have the unit of CM, concentration the units of G/CM$^3$, dispersivity the unit of CM, distribution coefficient for linear sorption the units of CM$^3$ /G, and so on.

A special note on the unit for concentration. Sometimes, it is more convenient to work with relative concentration. In that case, all concentrations input into the model can be scaled according to the maximum concentration (Co) of either aquifer or fluid sources. Subsequently, the model simulates the changes in the relative concentration (C/Co).

It should be emphasized that the unit names entered are used for identification purposes only, and do not affect the model simulation results in any way.

## 6.3 INTERFACE WITH THE FLOW MODEL

MT3D is designed to be used in conjunction with a block-centered finite-difference flowmodel. This allows the user to construct and calibrate a flow model independently. Prior to running MT3D, the heads, fluxes across cell interfaces in all directions, and locations and flow rates of the various sinks/sources, as solved by the flow model, should be saved in an unforrnatted head and flow file. This file should be saved in such a way that it can be retrieved by MT3D correctly through the Flow Model Interface Package. Appendix B, Linking MT3D with a Flow Model, gives more detailed information on the structure and form of the unformatted head and flow file.

In many cases, the U. S. Geological Survey modular three-dimensional finite-difference groundwater flow model (MODFLOW) will be used for the head solution; a package has therefore been written for use with MODFLOW to save heads and flow terms needed by MT3D. T'he package is named LKMT and included in the disk labelled *Flow Model,* which contains a version of the MODFLOW program already incorporating the LKMT package. If it is preferred to use a version of MODFLOW other than the one included in the *Flow Model disk,* do the followmg to add the LKMT package mto MODFLOW:

1. Insert the statements in file LKMT.INC into the MODFLOW main program between the following two statements:

   ```
   CALL BAS10C (... )
   IF(CNVG .EQ. 0) STOP
   ```

   and recompile the main program. Then, compile file LKMT.FOR and link it with the rest of the MODFLOW files. Both files LKMT.INC and LKMT.FOR are included in the *Flow Model Disk.*

2. Insert a positive integer number in the 22nd element of the IUNIT array in the input file for the MODFLOW Basic Package. This instructs the MODFLOW program to save the unformatted heads and flow terms for use in MT3D. It also serves as the

unit number on which the heads and flow terms will be saved. If the IUNIT(22) is entered as zero, no file will be saved by the LKMT Package.

It should be pointed out that the MODFLOW program already has the option to save heads andcell-by-cell flow terms in unformatted files. However, the MODFLOW program does not calculate fluxes between constant-head cells, which are required in the MT3D transport model. Furthermore, the MODFLOW program writes all the sink/source terms using three-dimensional arrays, thereby taking larger disk space than necessary. For these reasons, the MT3D program does not use the unformatted flow and cell-by-cell flow files in the forms saved by invoking the MODFLOW output control options.

## 6.4 INPUT INSTRUCTIONS FOR THE BASIC TRANSPORT PACKAGE

Input to the Basic Transport Package is read on unit 1, which is preset in the main program. Since the BTN Package is needed for every simulation, this input file is always required.

FOR EACH SIMULATION:

A1 Record: HEADNG(1)
Format: A80
HEADNG(1) is the first line of any title or heading for the simulation run. The line should not be longer than 80 characters.

A2 Record: HEADNG(2)
Format: A80
HEADNG(2) is the second line of any title or heading for the simulation run. The line should not be longer than 80 characters.

A3 Record: NLAY, NROW, NCOL, NPER
Format: 4110
NLAY is the total number of layers;
NROW is the total number of rows;
NCOL is the total number of columns; and
NPER is the total number of stress periods.

A4 Record: TUNIT, LUNIT, MUNIT
Format: 3A4
TUNIT is the name of unit for time, such as DAY or HOUR;
LUNIT is the name of unit for length, such as FT or CM;
MUNIT is the name of unit for mass, such as LB or KG.
These names are used for identification purposes only, and do not affect the model outcome.

A5 Record: TRNOP(10)
(ADV DSP SSM RCT XXX XXX XXX XXX XXX XXX)
Format: 10L2

TRNOP array contains logical flags for major transport options.
TRNOP(L) to (4) corresponds to Advection, Dispersion, Sink & Source Mixing, and Chemical Reaction Options, respectively. If any of these options is used, enter its corresponding TRNOP element as T, otherwise as F. TRNOP(5) to (10) are not used in the current version.

A6 Record: LAYCON(NLAY)
Format: 40I2
LAYCON is the model layer-type code. Enter one value for each layer. Enter LAYCON in as many lines as necessary if NLAY>40.
If LAYCON=0, the model layer is confined.
If LAYCON…0, the model layer is either unconfined or convertible between confined and unconfined. (Note that this corresponds to the LAYCON values of 1, 2, and 3 in MODFLOW; however, there is no need to distinguish between these layer types in the transport simulation.)

A7 Array: DELR(NCOL)
Reader: RARRAY
DELR is the cell width along rows (or ) *x*). Enter one value for each column in the grid.

A8 Array: DELC(NROW)
Reader: RARRAY
DELC is the cell width along columns (or ) *y*). Enter one value for each row in the grid.

A9 Array: HTOP(NCOL,NROW)
Reader: RARRAY
HTOP is the top elevation of cells in the first layer relative to the same datum as the heads. If the first layer is unconfined, HTOP can be set most conveniently to a uniform elevation above the water table (Fig. 6.2a). Note that the concentration for cells in the first layer is calculated at nodes assumed to be midway between HTOP and the bottom of the first layer.
HTOP should not be set much higher than the water table. If the first layer is confined, then, HTOP is equal to the bottom elevation of the confining unit overlying the first layer (Fig. 6.2b).

A10 Array: DZ(NCOL,NROW) (one array for each layer in the grid)
Reader: RARRAY

DZ is the cell thickness in each layer. DZ is a three-dimensional array. The input to three-dimensional arrays is handled as a series of two-dimensional arrays with one array for each layer, entered in the sequence of layer 1, 2, .... NLAY. The thickness of the first layer should be entered as the difference between HTOP and its bottom elevation. Under most circumstances, the grid is discretized into horizontal layers so that HTOP for the first layer and DZ within each layer are uniform (see Fig. 6.3a). However, if a distorted grid in the vertical direction is used, then, both HTOP and DZ are different for cells within the same layer (see Fig. 6.3b).

A11 Array: PRSITY(NCOL,NROW) (one array for each layer)
Reader: RARRAY

PRSITY is the effective porosity of the porous medium for each cell of the grid.

A12 Array: ICBUND(NCOL,NROW) (one array for each layer)
Reader: IARRAY

ICBUND is the boundary indicator array for the concentration field.

If ICBUND=0, then the cell is an inactive concentration cell. Note that no-flow or dry cells are automatically converted into inactive concentration cells. Furthermore, active head cells can be treated as inactive concentration cells to minimize the area needed for transport simulation, as long as the solute transport is insignificant near those cells.

If ICBUND<O, then the cell is a constant-concentration cell. The starting concentration remains the same at the cell throughout the simulation. Note that a constant-head cell *may or may not* be a constant-concentration cell.

If ICBUND>O, then the cell is a variable (active) concentration cell.

A13 Array: SCONC(NCOL,NROW) (one array for each layer)
Reader. RARRAY

SCONC is the starting concentration at the beginning of the simulation.

A14 Record: CINACT
Format: F10.0

CINACT is the value for indicating an inactive concentration cell (ICBUND=0). Even if it is not anticipated to have inactive cells in the model, a value for CINACT still must be submitted.

A15 Record: IFMTCN, IFMTNP, IFMTRF, IFMTDP, SAVUCN
Format: I10, I10, I10, I10, L10

IFMTCN is a flag indicating whether the calculated *concentration* should be printed and also serves as a printing-format code if it is printed. The codes forprint-formats are the same as those listed in Table 6. 1.

If CN>0, concentration is printed in the wrap form (Fig. 6.4a).
<0, concentration is printed in the strip form (Fig. 6.4b).
=0, concentration is not printed.

IFMTNP is a flag indicating whether the *number of particles in each cell* (integers) should be printed and also serves as a printing-format code if they are printed. The convention is the same as that used for IFMTCN.

IFMTRF is a flag indicating whether the model-calculated *retardation factor* should be printed and also serves as a printing-format code if it is printed. The convention is the same as that used for IFMTCN.

IFMTDP is a flag indicating whether the model-calculated distance-weighted *dispersion coefficient* should be printed and also serves as a printing-format code if it is printed. The convention is the same as that used for IFMTCN.

SAVUCN is a logical flag indicating whether the concentration should be saved in a default unformatted file (MT3D.UCN) for a continuation run or for post-processing purposes.

If SAVUCN=T, the concentration will be saved in file MT3D.UCN. In addition, the model spatial discretization information will also be saved in another default file named MT3D.CNF, to be used in conjunction with MT3D.UCN for post-processing.

If SAVUCN=F, neither MT3D.UCN nor MT3D.CNF is created.

A16 Record: NPRS
Format: 110

NPRS is a flag indicating the frequency of the output, and also indicating whether the output frequency is specified in terms of total elapsed simulation time or the transport step number. Note that what are actually printed or saved is controlled by the input values entered in the preceding record (Record A15).

If NPRS>0, simulation results will be printed or saved at times as specified in record TIMPRS(NPRS) to be entered in the next record.

If NPRS=0, simulation results will not be printed nor saved except at the end of simulation.

If NPRS<0, simulation results will be printed or saved whenever the number of transport steps is an even multiple of NPRS.

(Enter A17 only if NPRS > 0)

A17 Record: TIMPRS(NPRS)
Format: 8F10.0
TIMPRS is the total elapsed time at which simulation results are printed to the standard output file or saved in the default unformatted concentration file MT3D.UCN.
If NPRS > 8, enter TIMPRS in as many lines as necessary.

A18 Record: NOBS
Format: I10
NOBS is the number of observation points at which the concentration will be printed or saved at every transport step in the default observation point file MT3D.OBS.

(Enter A19 NOBS times if NOBS > 0)

A19 Record: KOBS, IOBS, JOBS
Format: 3I10
KOBS, IOBS and JOBS are the cell indices (layer, row, column) in which the observation point or monitoring well is located and for which the concentration is to be printed or saved at every transport step in file MT3D.OBS. Enter one set of KOBS, IOBS, JOBS for each observation point.

A20 Record: CHKMAS
Format: L10
CHKMAS is a logical flag indicating whether a one-line summary of mass balance information for each transport step should be saved in the default file named MT3D.MAS for checking purposes
If CHKMAS=T, the mass balance information for each transport step will be saved in file MT3D.MAS
If CHKMAS=F, file MT3D.MAS is not created.

FOR EACH STRESS PERIOD:

A21 Record: PERLEN, NSTP, TSMULT
Format: F10.0, I10, F10.0
PERLEN is the length of the current stress period.
NSTP is the number of time steps in the current stress period.
TSMULT is the multiplier for the length of successive time steps.
If TSMULT>0, the length of each time step within the current stress period is calculated using the geometric progression as in MODFLOW.

Note that PERLEN, NSTP and TSMULT must be the same as those used in the flow model except in steady state simulations.

If TSMULT:50, the length of time steps within the current stress period is read from a record TSMULT(NSTP) (see Record A22 below). This option is needed in case the length of time steps in the head solution is not based on a geometric progression in a flow model other than MODFLOW.

(Enter A22 if TSMULT ...0)

A22 Record: TSLNGH(NSTP)
Format: 8F10.0

TSLNGH provides the length of time steps in the current stress period. This record is needed only if the length of time steps for the head solution is not based on a geometric progression. Enter TSLNGH in as many lines as necessary if NSTP>8.

A23 Record: DTO, MXSTRN
Format: F10.0, I10

DT0 is the user-specified transport stepsize. The program win always calculate a maximum transport stepsize which meets the various stability criteria. Setting DT0 to zero or a negative value causes the model-calculated transport stepsize to be used in the simulation. However, the model-calculated DT0 may not always be optimal. In this situation, DT0 should be adjusted to find a DT0 which leads to the best results. If DT0 is given a value greater than the model-calculated stepsize, the model-calculated stepsize, instead of DT0 will be used in the simulation.

MXSTRN is the maximum number of transport steps allowed for one time step (of the head solution). If the number of transport steps within one time step exceeds MXSTRN, the simulation is terminated.

Fig. 6.2. Illustration of array HTOP for unconfined and confined aquifer layers.

Fig. 6.3. Arrays HTOP and DZ for different vertical discretization schemes.

Fig. 6.4. Illustration of wrap and strip forms of printed output for a layer containing 7 rows and l7 columns. (After McDonald and Harbaugh, 1988).

## 6.5 INPUT INSTRUCTIONS FOR THE ADVECTION PACKAGE

Input to the Advection Package is read on unit 2, which is preset in the main program. The input file is needed only if the Advection Package is used; however, this package is needed under almost all circumstances.

FOR EACH SIMULATION:

B1 Record: MIXELM, PERCEL, MXPART
Format: I10, F10.0, I10

MIXELM is a flag indicating the advection solution scheme.
If MIXELM=1, the Method Of Characteristics (MOC) is used.
=2, the Modified Method Of Characteristics (MMOC) is used.
=3, the Hybrid MOC/MMOC (HMOC) is used.
=0, the upstream finite difference method is used.

PERCEL is the Courant number, or number of cells any particle win be allowed to move in any direction in one transport step. PERCEL is used to calculate the maximum allowed stepsize for particle tracking. This stepsize is then compared with other stability criteria, if any, to determine an appropriate stepsize to be used in the simulation. Generally, 0.5#5PERCEL# l. However, values in excess of 1 can be used if the higher-order particle tracking method is used throughout the grid. Furthermore, because all cells in the entire grid are checked when calculating the maximum allowed stepsize for particle tracking, there may be a few cells where a particle will move more than one cell's length with PERCEL>1, while a particle will only move a fraction of a cell elsewhere. If these cells are outside the area of interest, setting PERCEL>1 will not result in inaccuracy. (Note that if MIXELM=0, i.e., using upstream finite-difference method for solving advection, PERCEL must not exceed 1.)

MXPART is the maximum number of total moving particles allowed, and is used only when MIXELM= 1 or 3.

(Enter B2 if MDCELM=1, 2 or 3)

B2 Record: ITRACK, WD
Format: I10, F10.0

ITRACK is a flag indicating which particle tracking algorithm is selected.
If ITRACK=1, thefirst-order Euler algorithm is used;
=2, the fourth-order Runge-Kutta algorithm is used,
=3, the Runge-Kutta algorithm is used in sink/source cells and the cells next to sinks/sources while the Euler algorithm is used elsewhere.

WD is a concentration weighting factor between 0 and 1. The value of 0.5 is normally a good choice. This number can be adjusted to achieve better mass balance. Generally, it can be increased toward 1 as advection becomes more dominant.

(Enter B3 ff MIXELM=1 or 3)

B3 Record: DCEPS, NPLANE, NPL, NPH, NPMIN, NPMAX, SRMULT

Format: F10.0, I10, I10, I10, I10, I10, F10.0

DCEPS is a small relative concentration gradient (DCCELL), such as $10^{-5}$, which is considered to be negligible.

NPLANE is a flag indicating whether the random or fixed pattern is selected for initial placement of moving particles.

If NPLANE=O, the the random pattern is selected for initial placement. particles are distributed randomly by calling a random number generator in both the horizontal and vertical directions (refer to Fig. 4.9b). This option generally leads to smaller mass balance discrepancy in nonuniform or diverging/converging flow fields.

If NPLANE>O, the fixed pattern is selected for initial placement. The value of NPLANE serves as the number of vertical "planes" on which initial particles are placed within each cell block (refer to Fig. 4.9a). This fixed pattern works well in relatively uniform flow fields. For two-dimensional simulations in plan view, set NPLANE=1. For cross sectional or three-dimensional simulations, NPLANE=2 is normally adequate. Increase NPLANE if more resolution in the vertical direction is desired.

NPL is number of initial particles per cell to be placed at cells where DCCELL#DCEPS. Generally, NPL can be set to 0 since advection is insignificant under the condition DCCELL#DCEPS. Setting NPL equal to NPH causes a uniform number of particles to be placed in every cell over the entire gdd (i.e., the uniform approach).

NPH is number of initial particles per cell to be placed at cells where DCCELL>DCEPS. The selection of NPH depends on the nature of the flow field and also the computer memory limitation. Generally, use a smaller number in relatively uniform flow fields and a larger number in relatively nonuniform flow fields. However, values exceeding 16 in two-dimensional simulation or 32 in three-dimensional simulation are rarely necessary. If the random pattern is chosen, NPH particles are randomly distributed within the cell block. If the fixed pattern is chosen, NPH is divided by NPLANE to yield the number of particles to be placed per vertical plane, which is rounded to one of the values shown in Fig. 6.5 NPMIN is the minimum number of moving particles allowed per

cell. If the number of particles in a cell at the end of a transport step is fewer than NPMIN, new particles are inserted into that cell to maintain a sufficient number of particles. NPMIN can be set to 0 in relatively uniform flow fields, and a number greater than zero in diverging/converging flow fields. Generally, 0# NPMIN# 4 is adequate.
NPMAX is the maximum number of particles allowed per cell. If the number of particles in a cell exceeds NPMAX, particles are removed from that cell until NP is met. Generally, NPMAX can be set to a value approximately twice the value of NPH.
SRMULT is a multiplier for the particle number at source cells (SRMULT$ l ). In most cases, SRMULT=1 is sufficient. However, better results may be obtained by increasing SRMULT.

(Enter B4 if MIXELM=2, or 3)
B4 Record: INTERP, NLSINK, NPSINK
Format: 3110
INTERP is a flag indicating the concentration interpolation method for use in the MMOC solution scheme. Currently, only linear interpolation is implemented. Enter INTERP=L.
NLSINK is a flag indicating whether the random or fixed pattern is selected for initial placement of particles to approximate sink cells in the MMOC scheme. The convention is the same as that for NPLANE.
NPSINK is the number of particles used to approximate sink cells in the MMOC scheme. The convention for is the same as that for NPH.

(Enter B5 if MDCELM=3)
B5 Record: DCHMOC
Format: F10.0
DCHMOC is the critical relative concentration gradient for controlling the selective use of either MOC or MMOC in the HMOC solution scheme.
The MOC solution is selected at cells where DCCELL>DCHMOC.
The MMOC solution is selected at cells where DCCELL< DCHMOC.

Fig. 6.5. Distribution of initial particies using the *fixed pattern*. If the fixed pattern is chosen, the number of particles placed per cell (NPL and NPH) is divided by the number of vertlcal "planes', or NPLANE, to yield the number of particles to be pieced on each vertical plane, which is then rounded to one of the values shown here.

## 6.6 INPUT INSTRUCTIONS FOR THE DISPERSION PACKAGE

Input to the Dispersion Package is read on unit 3, which is preset in the main program. The input file is needed only if the Dispersion Package is used in the simulation.

FOR EACH SIMULATION:

C1 Array: AL(NCOL,NROW) (One array for each layer).
Reader: RARRAY
AL is the longitudinal dispersivity ($\%_\mathrm{L}$) for each cell in the grid. (Unit: L).

C2 Array: TRPT(NLAY)
Reader: RARRAY
TRPT is the ratio of the horizontal transverse dispersivity ($\%_{TH}$) to the longitudinal dispersivity ($\%_L$) One value is specified for each layer.

C3 Array: TRPV(NLAY)
Reader: RARRAY
TRPV is the ratio of the vertical transverse dispersivity ($\%_{TV}$) to the longitudinal dispersivity ($\%_L$). One value is specified for each layer. Set TRPV equal to TRPT to use the standard isotropic dispersion model (equation 2.9 in Section 2.3.2). If TRPV is entered not equal to TRPT, the modified isotropic dispersion model is used (equation 2.10).

C4 Array: DMCOEF(NLAY)
Reader: RARRAY
DMCOEF is the effective molecular diffusion coefficient. (Unit: $L^2T^{-1}$). Set DMCOEF=0 if the effect of molecular diffusion is considered unimportant. One value is specified for each layer.

## 6.7 INPUT INSTRUCTIONS FOR SINK & SOURCE MIXING PACKAGE

Input to the Sink & Source Mixing Package is read on unit 4, which is preset in the main program. The input file is needed if any sink or source option is used in the flow model, including the constant-head or general-head-dependent boundary conditions. The classification of the sink/source type used in MT3D is the same as that used by MODFLOW (McDonald and Harbaugh, 1988).

## FOR EACH SIMULATION:

Dl Record: FWEL, FDRN, FRCH, FEVT, FRIV, FGHB
Format: 6L2

FWEL is a logical flag for the Well option;
FDRN is a logical flag for the Drain option;
FRCH is a logical flag for the Recharge option;
FEVT is a logical flag for the Evapotranspiration option;
FRIV is a logical flag for the River option; and
FGHB is a logical flag for General-Head-Dependent Boundary option.

If any of these options is used in the flow model, its respective flag must be set to T, otherwise, set to F.

D2 Record: MXSS
Format: I10

MXSS is the maximum number of all point sinks and sources simulated in the flow model. Point sinks and sources include constant-head cells, wells, drains, rivers, and general-head-dependent boundary cells. Recharge and evapotranspiration are treated as areally distributed sinks and sources; thus, they should not be counted as point sinks and sources. MXSS should be set close to the actual number of total point sinks and sources in the flow model in order to minimize the computer memory allocated to store sinks and sources.

## FOR EACH STRESS PERIOD:

(Enter D3 if FRCH=T)

D3 Record: INCRCH
Format: I10

INCRCH is a flag indicating whether an array containing the concentration of recharge fluxwill be read for the current stress period.

If INCRCH>O, an array containing the concentration of recharge flux will be read.

<O, the concentration of recharge flux will be reused from the last stress period. If INCRCH<O is entered for the first stress period, the concentration of recharge flux is set to zero by default.

(Enter D4 if FRCH=T and INCRCH $\geq$ 0)

D4 Array: CRCH(NCOL,NROW)
Reader: RARRAY

CRCH is the concentration of recharge flux. If the recharge flux is positive, the recharge acts as a source whose concentration can be specifled as desired. If the recharge flux is negative, the recharge acts as a sink (or discharge) whose concentration is always set equal to the concentration of the aquifer at the cell where discharge occurs. Note that the location and flow rate of recharge/discharge are obtained from the flow model directly through the unformatted head and flow file.

(Enter D5 if FEVT=T)

D5 Record: INCEVT
Format: I10

INCEVT is a flag indicating whether an array containing the concentration of evapotranspiration flux will be read for the current stress period.

If INCEVT $ 0, and array containing the concentration of evapotranspiration flux will be read.
<0, the concentration of evapotranspiration flux will be reused from the last stress period.

(Enter D6 if FEVT=T and INCEVT $ 0)

D6 Array: CEVT(NCOL,NROW)
Reader: RARRAY

CEVT is the concentration of evapotranspiration flux. Evapotranspiration is the only sink whose concentration can be specified externally. Note that the concentration of a sink cannot be greater than that of the aquifer at the sink cell. Thus, if the sink concentration is specified greater than that of the aquifer, it is automatically set equal to the concentration of the aquifer. Note that the location and flow rate of evapotranspiration are obtained from the flow model directly through the unfonmtted head and flow file.

D7 Record: NSS
Format: I10

NSS is the number of point sources whose concentrations need to be specified. Unspecified point sources are assumed to have a zero concentration by default.
(Note that the concentration of point sinks are always set equal to the concentration of the aquifer).

(Enter D8 if NSS>O)

| | | | | | |
|---|---|---|---|---|---|
| D8 Record: | KSS, | ISS, | JSS, | CSS, | ITYPE |
| Format: | I10, | I10, | | I10, | F10.0,I10 |

KSS, ISS, JSS are the cell indices (layer, row, column) of the point source for which a concentration is to be specified. CSS is the specified concentration. E is an integer number indicating the type of the point source as listed below. Enter one record for each point source of specified concentration. Note that the location and flow rate of point sources/sinks are obtained from the flow model directly through the unformatted head and flow file.

ITYPE =1, constant-head cell;
=2, well;
=3, drain;
=4, river;
=5, general-head-dependent boundary cell.

## 6.8 INPUT INSTRUCTIONS FOR THE CHEMICAL REACTION PACKAGE

Input to the Chemical Reaction Package is read on unit 5, which is preset in the main program. The input file is needed only if a sorption isotherm or a first-order rate reaction (decay or biodegradation) is simulated.

FOR EACH SIMULATION:

E1 Record: ISOTHM, IREACT
Format: 2I10

ISOTHM is a flag indicating whether, or if any, which sorption type is simulated.

If ISOTHM =l, Linear isotherm is simulated.
=2, Freundlich isotherm is simulated.
=3, Langmuir isotherm is simulated.
=0, no sorption isotherm is simulated.

IREACT is a flag indicating whether the first-order rate reaction is simulated.

If IREACT =1, radioactive decay or biodegradation is simulated.
=0, no first-order rate reaction is simulated

(Enter E2 if ISOTHM>0)

E2 Array: RHOB(NLAY)
Reader: RARRAY

RHOB is the bulk density of the porous medium in the aquifer. (Unit: $ML^{-3}$). One value is specified for each layer.

(Enter E3 if ISOTHM>O)

E3 Array: SP1 (NLAY)

Reader: RARRAY

SP1 is the first sorption constant. One value is specified each layer. The use of SP 1 depends on the type of sorption selected (i.e., ISOTHM).

For linear sorption, SP1 is the distribution coefficient ($K_d$). (Unit: $L^3M^{-1}$).

For Freundlich sorption, SP1 is the Freundlich sorption equilibrium constant ($K_f$). (Unit depends on the Freundlich exponent *a*).

For Langmuir sorption, SP1 is the Langmuir sorption equilibrium constant ($K_1$). (Unit: $L^3M^{-l}$).

(Enter E4 if ISOTHM>O)

E4 Array: SP2(NLAY)

Reader: RARRAY

SP2 is the second sorption constant. One value is specified for each layer. The use of SP2 depends on the type of sorption selected (i.e., ISOTHM).

For linear sorption, SP2 is not used, but still must be entered.

For Freundlich sorption, SP2 is the Freundlich exponent (*a*).

For Langmuir sorption, SP2 is the total concentration of sorption sites available ($\overline{S}$). (Unit: $MM^{-1}$).

(Enter E5 ff IREACT>0)

E5 Array: RC1(NLAY)

Reader: RARRAY

RC1 is the first-order rate constant for the dissolved phase. (Unit: $T^{-1}$). One value is specified for each layer.

(Enter E6 if IREACT >0 )

E6 Array: RC2(NLAY)

Reader: RARRAY

RC2 is the first-order rate constant for the sorbed phase. (Unit: $T^{-l}$). One value is specified for each layer. Generally, if the reaction is radioactive decay, SP2 should be set equal to SP1. However, for certain types of biodegradation, SP2 may be different from SP1.

## 6.9 START OF A SIMULATION RUN

There are two ways to start a simulation run. The first method is simply to type the name of the executable file. The program will prompt the user for the names of various input and output files. An example is given below, where "C:\>" is the command prompt and "MT3D" is the name of the executable file of the MT3D program:

```
C: \>MT3D
```

```
                              M T 3 D
             A Modular Three-Dimensional Transport Model
       For Simulation Advection, Dispersion and Chemical Reactions
              of Contaminants in Groundwater Systems

Enter Name for Standard Output File:                MT3D.OUT
Enter Name for Basic Transport Input File:          BTN.INP
Enter Name for Advection Input File:                ADV. INP
Enter Name for Dispersion Input File:               DSP.INP
Enter Name for Sink & Source Input File:            SSM.INP
Enter Name for Chemical Reaction Input File:        RCT.INP
Enter Name for Unformatted Head & Flow File:        MOD.FLO
Print out Heads and Flow  Terms for Checking (Y/N)? N

STRESS PERIOD NO.        1
TIME STEP NO.       1
FROM TIME = 0.00000           TO      100.00
Transport Step:      10    step size: 10.000          Tota1 Elapsed Time: 100.000
Program Completed.
```

The second method is to create a response file which contains the names of input and output files in the order required by the program. The content of such a response file (RUN.RL) for the example shown above would be as follows:

```
MT3D.OUT
BTN.  INP
ADV.  INP
DSP.INP
SSM.  INP
RCT.  INP
MOD.FLO
N
```

Then, at the command prompt,

```
C:\> MT3D  <  RUN.FIL
```

## 6.10 CONTINUATION OF A PREVIOUS SIMULATION RUN

Sometimes it may be necessary to break a long simulation run into several shorter ones. For example, if the flow model has many stress periods and time steps, the unformatted head and flow file generated by the flow model can be quite large. If there is not enough disk space, one has to break the simulation time into several intervals, with each interval having a separate head and flow file. Then, one needs to run the transport model once for each interval of the flow solution.  The continuation of a previous simulation run in the MT3D transport model is imiiar to the continuation of a flow simulation in the MODFLOW flow model.

First, save the concentrations from the final step of the preceding run on the default unformatted file MT3D.UCN. Next, re-name the file and use it as the starting concentration flle for the next run. (If there is more than one step of concentrations saved in the MT3D.UCN file, extract the concentrations at the last step using a program called SAVELAST included in the *Postprocessing Program Disk.)* The array reader which reads the starting concentrations (RARRAY) is capable of reading a model-generated unformatted concentration file with no modification.  Because mass budget terms are always set to zero at the start of a simulation run, the printed budget on a simulation run represents only that single run.  Therefore, if a total budget for a series of continuation runs is desired, the totals from each run can be added externally.  Similarly, the model program keeps track of simulation time only for single simulation runs; total simulation time for a series of continuation runs must be calculated externally by adding the simulation times of each run.

# Chaper 7
# VERIFICATION AND APPLICATION

In this chapter, the accuracy of theMT3D transport model is demonstrated through its use in solving several relatively simple problems for which analytical solutions are available. The applicability and flexibility of the transport model in solving more complicated field problems are also demonstrated using two typical examples. All files required to run these test problems are included in the *Example Disk.* It is recommended that the users spend some time studying and running these examples to become familiar with the various simulation options and input/output structures of the MT3D model before applying it to solve their own problems.

## 7.1 ONE-DIMENSIONAL TRANSPORT IN A UNIFORM FLOW FIELD

A relatively complete set of one-dimensional analytical solutions for solute transport involving advection, dispersion and some simple chemical reactions in a steady-state uniform flow field is available in Van Genuchten and Alves (1982). The problem considered in this section involves the following initial and boundary conditions:

$$\begin{array}{ll} C(x,0) = 0 & \\ C(0,t) = C_0 & t > 0 \\ \dfrac{\partial C}{\partial x}(\infty,t) = 0 & t > 0 \end{array}$$

A numerical model consisting of 101 columns, 1 row and 1 layer was used to solve the problem for comparison with the analytical solution for the same initial and boundary conditions as presented in Van Genuchten and Alves (1982). The model parameters used in the simulation are listed below:

Cell width along rows ( ) *x*) = 10 ft
Cell width along columns ( ) *y*) = 1 ft
Layer thickness ( ) *z*) = 1 ft
Groundwater seepage velocity (*v*) = 0.24 ft/day
Porosity (2) = 0.25
Simulation time (*t*) = 2000 days

The cell at the first column was treated as a constant concentration cell with a relative concentration of 1. Four simulation runs were made using different values of dispersivity, "$_L$ retardation factor, *R*, and decay rate constant, 8 as follows:

| | | | |
|---|---|---|---|
| Case 1: "$_L$ = 0, | R = 0, 8 = 0 | | Advection only. |
| Case 2: "$_L$ = 10*ft*, | R = 0, 8 = 0. | | Advection and dispersion. |
| Case 3: "$_L$ = 10*ft*, | R = *5*, 8 = 0. | | Advection, dispersion and sorption. |
| Case 4: "$_L$ = 10*ft*, | R = 5, 8= 0.002*day*$^{-1}$ | | Advection, dispersion, sorption and decay. |

Note that in this example the linear sorption isotherm was assumed and that the retardation factor was entered into the model by specifying a uniform bulk density of the porous medium and a uniform distribution coefficient of the linear sorption.

Cases 1 and 2 were simulated using the MOC option with these solution parameters: DCEPS=10$^{-5}$, NPL=0, NPH=4, NPMIN=0, NPMAX=10. These parameters imply that no particle (i.e., NPL=0) is placed in cells where the relative concentration gradient (DCCELL) is equal or less than 10$^{-5}$, considered negligible; and 4 particles (i.e., NPH=4) are inserted in cells where DCCELL> 10$^{-5}$. Since NPMIN=0, new particles are added only after a cell where DCCELL>DCEPS becomes void of any particle. With the one-dirnensional uniform flow field, it is only necessary to place particles in one plane vertically with a fixed pattern. An excellent match between the numerical and analytical solutions for both cases was obtained (Fig. 7. la). Note that no numerical dispersion is inuwuced even for the pure advection problem (Case 1).

Cases 3 and 4 were simulated using the MMOC option as advection becomes less important in these two cases. The simulation results for Cases 3 and 4 are plotted in Fig. 7.1b, and show excellent agreement with the analytical solution.

Fig. 7.1. Breakthrough curves for the one-dimensional test problem.

## 7.2 TWO-DIMENSIONAL TRANSPORT IN A UNIFORM FLOW FIELD

An analytical solution for two-dimensional transport of solute injected continuously from a point source in a steady-state uniform flow field is given by Wilson and Nfiller (1978). The analytical solution is applicable only under the assumption that

1) the aquifer is relatively thin, so that instantaneous vertical mixing can be assumed;

2) the injection rate is insignificant compared with the ambient uniform flow.

A numerical model consisting of 46 columns, 31 rows and 1 layer was constructed to simulate a test problem with approximately the same assumptions for comparison with the analytical solution of Wilson and Miller (1978). The configuration of the test problem is shown in Fig. 7.2(a) and the model parameters used in the simulation are listed below:

Cell width along rows ( ) *x*) = 10 m
Cell width along columns ( ) *y*) = 10 m
Layer thickness ( ) *z*) = 10 m
Groundwater seepage velocity (*v*) = 1/3 m/day
Porosity (2) = 0.3
Longitudinal dispersivity = 10 m
Ratio of transverse to longitudinal dispersivity = 0.3
Volumetric injection rate = 1 m$^3$/day
Concentration of the injected water = 1000 ppm
Simulation time (*t*) = 365 days

The hybrid MOC/MMOC, or HMOC option was used in the simulation, with DCHMOC set to $10^{-3}$ and the rest of the solution parameters as follows:

(for the MOC scheme):

DCEPS=$10^{-5}$, NPLANE=1, NPL=0, NPH=9, NPMIN=0, NPMAX=16

(for the MMOC scheme):

INTERP=l NLSINK=1, NPSINK=9

Thus, in the solution process, the MOC scheme was automatically selected in cells where DCCELL>$10^{-3}$ ; and the MMOC scheme was automatically selected in cells where DCCELL # $10^{-3}$. When the MOC scheme was used, 9 particles were placed in cells with a fixed pattern on one vertical plane (NPLANE=l) where DCCELL is greater than the specified negligible limit. When the MMOC scheme was used, 1 fictitious particle was placed at the nodal point for backward tracking except at a sink cell where 9 particles were placed (i.e., NPSINK=9) on one (1) vertical plane within the sink cell block (i.e., NLSINK=l). The option selected for particle tracking is ITRACK=3. In other words, the fourth-order Runge-Kutta method is used in the vicinity of the point source whereas the first Euler method is used elsewhere.

The contour map of the concentration field at the end of the 365-day simulation period obtained for this test problem is shown in Fig. 7.2. The numerical solution agrees well with the analytical solution.

The HMOC option offered some advantage over either MOC or MMOC option alone in this example. The MMOC option alone can lead to some numerical dispersion with the Peclet number (Pe) equal to 1 along the x-direction. The MOC option alone requires about 7000 particles at the end of the 1-year simulation period. One the other hand, the HMOC option virtually eliminates the numerical dispersion while using approximately half the total number of moving particles required by the MOC option alone. The DCHMOC criterion is a empirical value, and requires some trial and error before an optimal number may be determined. However, as found in this and subsequent test examples, values between 0.01 and 0.001 are normally adequate.

Fig. 7.2. Comparison of the numerical and analytical solutions for two-dimensional from a point source in a uniform flow field.

## 7.3 TWO-DIMENSIONAL TRANSPORT IN A RADIAL FLOW FIELD

The problem considered in this section concerns the two-dimensional transport of solute injected from a fully penetrating well. The assumptions for this problem are:

1) the injection rate of the well is constant;
2) the ambient groundwater velocity is negligible relative to the velocity created by the injection;
3) the aquifer is homogeneous, isotropic, and infinite in areal extent; and
4) the flow field is steady-state.

The initial and boundary conditions for this problem are

$$
\begin{aligned}
&C\,(r\,,0) = 0 && \\
&C\,(r_w\,,t) = C_0 && t > 0 \\
&\left.\frac{\partial C}{\partial r}\right|_{r \to \infty} && t > 0
\end{aligned}
$$

where $r_w$ is the well radius. An approximate analytical solution for this problem is given by Moench and Ogata (1981) and available in a computer program (LTIRD) provided by Javandel et. al. (1984).

A numerical model consisting of 31 columns, 31 rows and 1 layer was used to solve this problem for comparison with the analytical solution of Moench and Ogata (1981). The model parameters used in the simulation are listed below:

Cell width along rows ( ) *x*) = 10 ft
Cell width along columns ( ) *y*) = 10 ft
Layer thickness ( ) *z*) = 1 ft

Porosity (2) = 0.3
Longitudinal dispersivity = 10 ft
Ratio of transverse to longitudinal dispersivity = 1
Simulation time (*t*) = 27 days

The cell at column 16 and row 16 was simulated as the constant concentration cell with a relative concentration of 1. Again, the hybrid MOC/MMOC (or HMOC) option was used for the simulation with DCHMOC set to $10^{-2}$ and the rest of the solution parameters as follows:

(for the MOC scheme):

DCEPS=$10^{-5}$, NPLANE=1, NPL=0, NPH=16, NPMIN=2, NPMAX=30

(for the NMOC scheme):

INTERP=1, NLSINK=l, NPSINK=9

The solution parameters shown above are similar to those used in the preceding example except that in the current example NPH was increased to 16 and NPMIN and NP to 2 and 30, respectively. Generally, the number of moving particles per cell in a diverging/converging flow field should be greater than that in a relatively uniform flow field. This is because in a diverging/converging flow field, more particles are needed to maintain the same resolution because of the spreading of particles in different directions. Furthermore, in a diverging/converging flow field, NPMIN should normally be entered with a value greater than 0 so that new particles can be added to source cells before those cells become depleted of particles, thus avoiding large mass balance discrepancies. The optimal value for NPMIN in a particular problem can be determined by adjusting it until the smallest mass balance discrepancy is achieved. It is found that values between 1 and 4 can generally lead to satisfactory results.

The contour map of the simulated concentration field at the end of the 27-day simulation period is plotted in Fig. 7.3(a). The contour lines form approximately symmetric circles around the source, an indication that the numerical model can simulate radial advection and dispersion accurately even though it is written in the Cartesian coordinate system. The distribution of the simulated concentrations along the x-axis from the point source to the model edge is plotted in Fig. 7.3(b) and is nearly identical to that of the analytical solution.

Fig. 7.3. Comparison of the numerical and analytical solutions for two-dimensional from a point source in a radial flow field.

## 7.4 CONCENTRATION AT AN INJECTION/EXTRACTION WELL

Injection/extraction wells are commonly used in practice to contain and clean up contaminants in groundwater. Therefore, in many practical transport simulations involving evaluation of the effectiveness of remedial alternatives, it is important for the transport model to have the ability to approximate closely the concentrations at injection/extraction wells.

A problem involving an injection/pumping cycle for a fully penetrating well in a confined aquifer was used to test this capability of the MT3D transport model. Water of a constant concentration ($C_0$) was injected into the well. After a certain period of time ($t_1$), the flow was reversed, and the contaminated water was pumped out. Assuming that the flow field reaches steady state instantaneously after the injection and pumping cycles start, an approximate analytical solution for this problem is given by Gelhar and Collins (1971).

A numerical model consisting of 31 columns, 31 rows and 1 layer was used to simulate the concentration change at the injection/extraction well for comparison with the approximate analytical solution of Gelhar and Collins (1971). The model parameters used in the simulation were the same as those used by El-Kadi (1988) to test the U.S. Geological Survey two-dimensional solute transport model (Konikow and Bredehoeft, 1978) as listed below:

Cell width along rows ( ) $x$) = 900 ft
Cell width along columns ( ) $y$) = 900 ft
Layer thickness ( ) $z$)= 20 ft
Hydraulic conductivity of the aquifer = 0.005 ft/s
Porosity (2) = 0.3
Longitudinal dispersivity = 100 ft
Ratio of transverse to longitudinal dispersivity =1
Volumetric injection/extraction rate = 1 ft$^3$/s
Relative concentration of the injected water = 100 percent
Length of the injection period = 2.5 years
Length of the extraction period = 7.5 years

The MOC option was used in the simulation as the transport process is largely dominated by advection, with cell Peclet numbers in the vicinity of 10. The solution parameters for the MOC scheme are NPL=16, NPH=16, NPMIN=4 and NPMAX=30. Because NPL is set equal to NPH, a uniform distribution of 16 particles per cell was initialized over the entire grid. Initial particles were placed randon-fly within each cell block. The selection of the random pattern over the fixed pattern leads to a smaller mass balance discrepancy due to the strongly diverging/converging nature of the flow field. The fourth-order Runge-Kutta particle tracking algorithm was selected to increase the accuracy of the solution.

The breakthrough curve of concentration at the injection/extraction well is plotted in Fig. 7.4. The match between the numerical and analytical solutions is reasonably good despite the coarse grid (900 by 900 ft) and the strongly diverging/converging flow field. The mass balance discrepancy for this simulation at the end of the 10 year simulation period is about 1.0 percent and averages approximately 1.3 percent over the total 28 transport steps.

## 7.5 THREE-DIMENSIONAL TRANSPORT IN A UNIFORM FLOW FIELD

In Section 7.2, two-dimensional transport from a point source in a uniform flow field was considered under the assumption of a relatively thin aquifer and instantaneous vertical mixing. However, if the aquifer is thick and instantaneous vertical mixing cannot be assumed, the transport of solute away from the point source should be considered three dimensional. An analytical solution for three-dimensional transport with the same set of initial and boundary conditions as discussed in Section 7.2 is given by Hunt (1978).

A numerical model consisting of 21 columns, 15 rows and 8 layers was used to solve the three-dimension transport problem for comparison with the analytical solution of Hunt (1978). The point source was simulated at column 1, row 8, and layer 7. The model parameters used in the simulation are listed below:

Fig. 7.4. Concentration at the well during an injection/pumping cycle as calculated by the MT3D model and the analytical solution in a strongly diverging/converging flow field.

Cell width along rows ( ) *x*) = 10 ft
Cell width along columns ( ) *y*) = 10 ft
Layer thickness ( ) *z*) = 10 ft
Groundwater seepage velocity = 0.5 ft/day
Porosity (2) = 0.2
Longitudinal dispersivity = 10 ft
Ratio of horizontal transverse to longitudinal dispersivity = 0.3
Ratio of vertical transverse to longitudinal dispersivity = 0.3
Volumetric rates of injection = 0.5 $ft^3$/day
Relative concentration of the injected water = 100 percent
Simulation time (*t*) = 100 days

The HMOC option was used in the simulation with DCHMOC set equal $10^{-2}$ and the rest of the solution parameters as follows:

(for the MOC scheme):

DCEPS=$10^{-5}$, NPLANE=2, NPL=0, NPH=8, NPMIN=0, NPMAX=30

(for the MMOC scheme):

INTERP=1, NLSINK=2, NPSINK=8

In this example, initial particles were placed on two vertical planes (i.e., NPLANE=2) within each cell block, with 4 particles on each plane. For three-dimensional or cross sectional simulations, NPLANE=2 to 4 is normally adequate. Note that NPLANE is used only if the fixed pattern is selected for the initial particle placement (with the random pattern, the random number generator places particles randomly both horizontally and vertically with each cell block.)

The contours of relative concentration obtained in the simulation for layers 5, 6, and 7 at the end of the 100-day simulation period are plotted in Fig. 7.5, and show good agreement with those calculated by the analytical solution.

Fig. 7.5. Comparison of the numerical and analytical solutions for three-dimensional from a point source in a uniform flow field.

## 7.6 TWO-DIMENSIONAL TRANSPORT IN A HETEROGENEOUS AQUIFER

This section describes the application of the model to a test problem involving transport of contaminants in a two-dimensional heterogeneous aquifer. The problem was simulated to illustrate the applicability of the transport model to solve more complicated problems for which analytical solutions do not exist.

The configuration of the test problem is shown in Fig. 7.6. The flow domain is bounded by no-flow boundaries on the east and west sides. The north side is a constant-head boundary and the south side a specified-head boundary with hydraulic head dropping toward the west. Water of a constant concentration is injected into the aquifer through a fully penetrating well, while a pumping well located downstream removes solute mass from the aquifer. Between the injection and pumping wells there is a zone of a low hydraulic conductivity in which the hydraulic conductivity is three orders of magnitude smaller than that elsewhere in the simulated region. The parameters used in the simulation are listed below (also see Fig. 7.6):

Cell width along rows ( ) *x*) = 100 m
Cell width along columns ( ) *y*) = 100 m
Layer thickness ( ) *z*) = 10 m

Porosity (2) = 0.3
Longitudinal dispersive = 20 ft
Ratio of horizontal transverse to longitudinal dispersive = 0.2
Simulation time (*t*) = 1 year

The flow and transport models consist of 16 columns, 20 rows, and 1 layer. The boundary conditions for the transport model are no-mass flux boundaries on the east, west, and north borders of the model. The south border was treated as a line of point sinks taking mass out of the aquifer.

Fig. 7.6. Configuration of the heterogeneous aquifer simulated in the test problem.

The HMOC option was used in the transport simulation with DCHMOC set equal to 2xl0$^{-3}$ and the rest of the solution parameters as follows:

(for the MOC scheme):

DCEPS=10$^{-5}$, NPLANE=0, NPL=0, NPH=16, NPMIN=2, NPMAX=30

(for the MMOC scheme):

INT'ERP=1, NLSINK=0, NPSINK=16

Initial particles were distributed using the random pattern (NPLANE=0). The fourth-order Runge-Kutta algorithm (i.e., ITRACK=2) was selected to move all particles to ensure the accuracy of the particle tracking calculations in the heterogeneous aquifer. In the previous examples, the number of cells a particle was allowed to move in any direction (i.e., PERCEL) was always set equal to a value between 0.5 and 1.0. In other words, no particles were allowed to move more than one cell's length in any direction. However, in the current example, PERCEL=1.5 was found to give better mass balance results than PERCEL=1.0, with all other parameters held the same.

T'he simulated concentration field at the end of 1-year simulation period is plotted in Fig. 7.7. The mass balance discrepancy for this simulation is shown in Fig. 7.8. While the discrepancy tends to be relatively large at early times, it decreases to near zero as simulation continues. The average for the full simulation (28 transport steps) is less than 0.3%, indicating that the mass injected into the aquifer is largely conserved.

It is interesting to compare Fig. 7.7 with Fig. 7.9 which shows the concentration field for this problem as simulated by the pure finite difference method. While the general patterns of these two simulated plumes are quite similar, it is clear that the pure finite difference solution introduces a certain amount of numerical dispersion, which causes artificial smearing of the plume.

Fig. 7.7. Distribution of solute concentrations as solved by the hybrid MOC/MMOC (HMOC) solution.

Fig. 7.8. Plot of the mass balance discrepancy error at each rt step for the test problem involving a heterogeneous aquifer.

Fig. 7.9. Distribution of solute concentrations as solved by the finite difference solution for comparison with those solved by the hybrid MOC/MMOC (HMOC)solution (Fig. 7.7).

## 7.7 A THREE-DIMENSIONAL FIELD APPLICATION

This section describes the application of the MT3D transport model to an actual field problem involving evaluation of the effectiveness of proposed groundwater remediation schemes; the discussion is intended to demonstrate the performance of the model in a representation of real world problems. The geologic setting of the site is illustrated in Fig. 7. 10. The aquifer is unconfined and consists mostly of medium-grained sand exhibiting two distinctive hydraulic conductivities, about 60 ft/day in the shallow zone and approximately 600 ft/day in the deeper zone. The recharge rate estimated for the site is 5 inches per year. The porosity value is approximately 30 percent. Several organic compounds have been detected in groundwater beneath the site. Among them is 1,2-dichloroethane (1,2-DCA), which is found over an area of more than 2200 feet by 1300 feet, with the maximum concentration exceeding 200 ppb.

A numerical model was developed for this site to investigate the effectiveness and performance of various remedial scenarios designed to clean up the aquifer. The model consisted of four layers in the vertical direction as shown in Fig. 7.10. In plan view, 61 rows and 40 columns were used (see Fig. 7.11). The boundaries were set sufficiently far away from the site to minimize their effect on flow and transport in the immediate vicinity of the site. Most of the cers were concentrated in the central part of the mesh, denoted ABCD in Fig. 7.11, in the area of the contaminant plume. The flow field was simulated using the MODFLOW flow model assuming the steady-state condition.

The present distribution of 1,2-dichoroethane (time=0) is shown in Fig. 7.12a. One of the scenarios for cleanup is to use 8 extraction wells (shown in the figure as squares labelled from Wl to W8) to pump contaminated groundwater out of the aquifer for treatment. The longitudinal dispersivity used for the modeling is 10 feet, with horizontal and vertical transverse dispersivities of 2 feet. A uniform retardation factor equal to 2 was calculated from the uniform bulk density and distribution coefficient selected. The proposed total extraction rate for the eight wells was about 700 gpm, all from layer 3.

The IMOC option was used in the transport simulation with DCHMOC set to $10^{-2}$ and the rest of the solution parameters as follows:

(for the MOC scheme):

DCEPS=$10^{-5}$, NPLANE=0, NPL=0, NPH=10, NPMIN=2, NP =30

(for the MMOC scheme):

INTERP=1, NLSINK=0, NPSINK=10

Initial particles were distributed using the random pattern (NPLANE=0). The random pattern was found to be superior to the fixed pattern in this application due to the nature of the flow field. The mixed first-order Euler and fourth-order Runge-Kutta algorithm (i.e., ITRACK=3) was selected for particle tracking in the heterogeneous aquifer. The Courant number (i.e., PERCEL) was set equal to 1.0. The concentration weighting factor (i.e., WD) entered was as 0.5.

The concentration distributions in layer 3 within area ABCD after 500, 750 and 1000 days from the time when pumping starts, as predicted by the MT3D transport model, are shown in Figs. 7.12b, 7.12c and 7.12d, respectively. The concentration breakthrough curves at pumping wells Wl, W4 and W6, which are located in the the northern end, middle point, and southern end of the plume, respectively, are plotted in Fig. 7.13. The mass balance discrepancy at the end of the 1000-day simulation period was about 2.7 percent, and averaged 3.8 percent over the 128 transport steps in the entire simulation.

Fig. 7.10. Setting and vertical discretization in the field example.

Fig. 7.11. Plan view of the finite difference mesh for the field example.

Fig. 7.12. Present distribution of the disolved l,2-DCA and the model-predicted concentration changes at selected times after pumping starts

Fig. 7.13. Concentration breakthrough curves at pumping wells W1, W4 and located at the northern end, middle area and southern end of the plume, respectively. (Concentrations are shown in the plot every five steps.)

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# Appendix A

# SPACE REQUIREMENTS

# Appendix A
## SPACE REQUIREMENTS

The elements of the X and IX arrays required by each package for a given problem are always printed by the model program every time it is run. They can also be calculated according to the formulas given below. Variables used in the formulas are defined as follows:

NCOL = the total number of columns;  
NROW= the total nuumber of rows;  
NLAY = the total umber of layers;  
NODES= NCOL*NROW*NLAY, the total number of cells in the model;  
MXSS = the number of all point sinks and sources present in the flow model, including constant-head and general-head-dependent boundary cells, but excluding recharge and evapotranspiration cells;  
MXPART= the maximum number of moving particles allowed;  
ND = the number of dimensions in the given problem (ND=l for a one-dimensional problem; 2 for a two-dimensional problem and 3 for a three-dimensional problem).

**A. BASIC TRANSPORT PACKAGE (BTN)**

I. X Array  
(ND+9)*NODES+2*NROW+2*NCOL

II. IX Array  
NODES+NLAY

**B. ADVECTION PACKAGE (ADV)**

I. X Array  
(ND+l)*MXPART

II. IX Array  
NODES

**C. DISPERSION PACKAGE (DSP)**

I. X Array  
(ND$^2$+1)*NODES+3*NLAY

II. DC Array  
None

**D. SINK & SOURCE MIXING PACKAGE (SSM)**

I. X Array  
6*MXSS  
If recharge is simulated, add 2*NROW*NCOL  
If evapotranspiration is simulated, add 2*NROW*NCOL

II. IX Array  
If recharge is simulated and NLAY>1, NROW*NCOL  
If evapotranspiration is simulated and NLAY>1, add NROW*NCOL

## E. CHEMICAL REACTION PACKAGE (RCT)

I. X Array

If sorption is simulated, 4*NLAY

If first-order rate reaction is simulated, add 2*NLAY

II. IX Array

None

# Appendix B

# LINKING MT3D WITH A FLOW MODEL

# Appendix B
## LINKING MT3D WITH A FLOW MODEL

The Flow Model Interface Package of MT3D reads the hydraulic heads, fluxes across cell interfaces in the row, column and layer directions, and locations and flow rates of the various sources and sinks from an unformatted file saved by the flow model used in conjunction with the MT3D transport model. If the U.S. Geological Survey modular flow model (MODFLOW) is used for the flow simulation, a package named LKMT, which is included in the *Flow Model Disk*, can be linked to the MODFLOW program to save the following information as explained in Section 6.2. If a flow model other than MODFLOW is used in the flow simulation, the flow model can be modified to save the heads and flow terms as instructed below.

FOR EACH TIME STEP OF THE HEAD SOLUTION:

Fl. Record: KPER, KSTP, NCOL, NROW, NLAY, LABEL
F2. Record: H(NCOL,NROW,NLAY)
KPER--the stress period number at which the head and flow terms are saved
KSTP--the time step number at which the head and flow terms are saved
NCOL, NROW, NLAY--number of columns, rows and layers
H--hyaulic heads. Heads at inactive cells must be set equal to l.E30.
LABEL--'HEAD', identifying character label for heads
(If NCOL=l, skip F3 and F4)
F3. Record: KPER, KSTP, NCOL, NROW, NLAY, LABEL
F4. Record: QX(NCOL,NROW,NLAY)
QX--volumetric fluxes between cells at cell interfaces along rows (or the x-axis). Positive in the direction of increasing J index.
LABEL='QXX', identifying character label for QX
(If NROW= 1, skip F5 and F6)
F5. Record: KPER, KSTP, NCOL, NROW, NLAY, LABEL
F6. Record: QY(NCOL,NROW,NLAY)
QY--volumetric fluxes between cells at cell interfaces along columns(or the y-axis). Positive in the direction of increasing I index.
LABEL='QYY', identifying character label for QYY
(If NLAY=1, skip F7 and F8)
F7. Record: KPER, KSTP, NCOL, NROW, NLAY, LABEL
F8. Record: QZ(NCOL,NROW,NLAY)
QZ--volumetric fluxes between cells at cell interfaces along layers (or the z-axis). Positive in the direction of increasing K index.
LABEL='QZZ', identifying character label for QZ
F9. Record: KPER, KSTP, NCOL, NROW, NLAY, LABEL, NCNH
NCNH--number of constant-head cells

LABEL='CNH', identifying character label for constant head

(If NCHN>0, there must be NCNH records of F10)

F10. Record: KCNH,ICNH,JCNH,QCNH

KCNH,ICNH,JCNH-cell indices of each constant-head cell

QCNH--volumetric net flow rate out of or into the constant-head cell, including exchange between constant-heads (this is different from the net flow rate calculated at a constant-head cell in MODFLOW). Positive if flow is out of the constant head cell, negative otherwise.

(If wells are not present in the flow model, skip F11 and F12)

F11. Record: KPER, KSTP, NCOL, NROW, NLAY, LABEL, NWEL

NWEL--number of wells

LABEL='WEL', identifying character label for well

(If NWERL>0, there must be records of F12)

F12. Record: KWEL,IWEL, JWEL,QWEL

KWEL,IWEL,JWEL--cell indices of each well

QWEL--volumetric flow rate of the well. Positive if into the cell, negative otherwise. (The same convention is followed by the remaining sink/source terms).

(If drains are not present in the flow model, skip F13 and F14)

F13. Record: KPER, KSTP, NCOL, NROW, NLAY, LABEL,NDRN

NDRN--number of drains

LABEL='DRN', identifying character label for drain

(If NDRN>0, there must be NDRN records of F14)

F14. Record: KDRN,IDRN,JDRN,QDRN

KDRN,IDRN,JDRN--cell indices of each drain

QDRN--volumetric flow rate of the drain

(If recharge is not present in the flow model, skip F15, F16 and F17)

F15. Record: KPER, KSTP, NCOL, NROW, NLAY, LABEL

LABEL--'RCH', identifying character label for recharge

(If NLAY= 1, skip F16)

F16. Record: IRCH(NCOL,NROW)

IRCH--layer indices of the recharge flux

F17. Record: RECH(NCOL,NROW)

RECH--volumetric rate of recharge

(If evapotranspiration is not present in the flow model, skip F18, F19, and F20)

F18. Record: KPER,KSTP,NCOL,NROW,NLAY,LABEL

LABEL--'EVT', identifying character label for evapotranspiration

(If NLAY=1, skip F19)

F19. Record: IEVT(NCOL,NROW)

IEVT--layer indices of the evapotranspiration flux

F20. Record: EVTR(NCOL,NROW)

EVTR--volumetric rate of evapotranspiration

(If rivers are not present in the flow model, skip F21 and F22)

F21. Record: KPER, KSTP, NCOL, NROW, NLAY, LABEL,NRIV

NRIV--number of rivers

LABEL='RIV', identifying character label for river

(If NRIV>0, there must be NRIV records of F22)

F22. Record: KRIV,IRIV,JRIV,QRIV

KRIV,IRIV,JRIVN--cell indices of each river

QRIV--volumetric flow rates of the river reaches

(If general-head-dependent boundaries not present in the flow model skip F23 and F24)

F23. Record: KPER, KSTP, NCOL, NROW, NLAY, LABEL,NGHB

(If NGHB>0, there must be NGHB records of F24)

F24. Record: KGHB,IGHB,JGHB,QGHB

KGHB,IGHB,JGHB--cell indices of each general-head-dependent boundary cell QGHB--volumetric flow rates of the general-head-dependent boundary cells

# Appendix C
# SAMPLE INPUT AND OUTPUT FILES

```
INPUT FILE TO BTN PACKAGE
-------------------------

3-D TRANSPORT MODEL FOR REMEDIAL DESIGN

(REFER TO SECTION 7.7)
         4            61           40             1
DAY   FT    UNDF
T  T  T  T                                                      NLAY,NROW,NCOL
    1 0 0 0 0 0                                                 LUNIT,TUNIT,MUNIT
       103            0.                          7             ADV,DSP,SSM,RCT
2000.00   1600.00   800.00   400.00   200.00   100.00           LAYCON
28*50                                                           ARRAY CONTROL-RECORD FOR DELR
100.00    200.00    400.00   800.00   1600.0   2000.00
          103         0.                          7
2000.00   2000.00   2000.00  1600.00  800.00                    DELR ENTERED IN FREE FOR M
400.00    200.00    100.00  45*50     l00.00   200.00           ARRAY CONTROL-RECORD FOR DELC
400.00    800.00    1600.00  2000.00  2000.00  2000.00
        0         780.
        0           25.00                                       DELC ENTERED IN FREE FORM
        0           25.00                                       HTOP, ENTERED AS A UNIFORM VALUE
        0           25.00                                       DZ-LAYER1, ENTERED AS A UNIFORM VALUE
        0           25.00                                       DZ-LAYER2
        0             .30                                       DZ-LAYER3
        0             .30                                       DZ-LAYER4
        0             .30                                       POROSITY-LAYER1
        0             .30                                       POROSITY-LAYER2
        0           1                                           POROSITY-LAYER3
        0           1                                           POROSITY-LAYER4
        0           1                                           ICBUND-LAYER1
        0           1                                           ICBUND-LAYER2
        0           0.                                          ICBUND-LAYER3
        99            .2(20F8.3)                                ICBUND-LAYER4
        99          1. (20F8.3)                                 SCONC-LAYER1
        0           0.                                          SCONC-LAYER2(READ FROM EXTERNAL FILE ON UNIT 99)
  -999.99                                                       SCONC-LAYER3(READ FROM  EXTERNAL FILE ON UNIT 99)
       8         2          0        0          T               SCONC-LAYER4
       1                                                        CINACT
     500                                                        IFMTCN, IFMTNP, IFMTRF, IFMTDP, SAVUCN
        8                                                       NPRS
        3         11        29                                  TIMPRS
        3         19        26                                  NOBS
        3         26        23                                  KOBS, IOBS, JOBS
        3         33        20
        3         40        17
        3         48        14
        3         48         9
        3         52        17
        T
    1000.           1        1.
      0.         1000                                           CHKMAS
                                                                PERLEN, NSTP, TSMULT
                                                                DTO, MXSTRN
```

```
INPUT FILE TO ADV PACKAGE
  -------------------------
       3          1.    75000
       3           .50
  1.e-5               0      0     10       2      30       1               MIXELM,PERCEL,MXPART
      1               0      8                                              ITRACK WD
    .01                                                                     DCEPS,NPLANE NPL NPH,NPMIN,NPMAX,SRMULT
                                                                            INTERP,NLSINK, NPSINK
                                                                            DCHMOC
```

```
INPUT FILE TO DSP PACKAGE
-------------------------

      0       10.
      0       10.
      0       10.                                                           AL-LAYER1, ENTERED AS A UNIFORM VALUE
      0       10.                                                           AL-LAYER3
      0       .20                                                           AL-LAYER3
      0       .20                                                           AL-LAYER4
      0        0.                                                           TRPT, ENTERED AS A UNIROM VALUE
                                                                            TRPV
                                                                            DMCOEF
```

```
INPUT FILE TO SSM PACKAGE
       -------------------------

  T  F  T  F  F  F
             2000
                1                                                           FWEL,FDRN,FRCH,FEVT,FRIV,FGHB
                0       0.                                                  MXSS
                0                                                           INCRCH
                                                                            CRCH, ENTERED AS A UNIFORM VALUE
                                                                            NSS
```

```
INPUT FILE TO RCT PACKAGE
-------------------------

      1        0
      0        .3
      0       1.                                                            ISOTHM IREACT
      0       1.                                                            RHOB, ENTERED AS A UNIFORM VALUE
                                                                            SP1
                                                                            SP2
```

```
M T 3 D
A Modular Three-Dimensional Transport Model
For Simulation of Advection, Dispersion and Chemical Reactions
of Contaminants in Groundwater Systems

M T    3-D  TRANS MODEL F0R REMEDIAL DESIGN
3 D     (REFER TO SECTION 7.7)

THE TRANSPORT MODEL CONSISTS OF          4 LAYER(S)       61 ROW(S)    41 COLUMN(S)
NUMBER OF STRESS PERI OD (S) I N SIMULA T ION    =       1
UNIT FOR TIME IS        DAY ;   UNIT FOR LENGTH IS    FT ;  UNIT FOR MASS IS UNDF
M AJOR TRAANSPORT COMPONENTS TO BE SIMULATED:
        1       ADVECTION
        2       DISPERSION
        3       SINK AND SOURCE MIXING
        4       CHEMICAL REACTIONS (DECAY AND/OR SORPTION)

BTN1  --  BASIC TRANPORT PACKAGE, VER  1.0,  AUGUST 1990,  INPUT READ FROM UNIT    1
        117322 ELEMENTS OF THE X ARRAY USED BY THE BTN PACKAGE
          9764 ELEMENTS OF THE IX ARRAY USED BY THE BTN PACKAGE

ADV1  --  ADVECTION PACKAGE, VER 1.0,  AUGUST  1990,     INPUT READ FRO14 UNIT 2
ADVECTION IS SOLVED WITH THE HYBRID  [MOC]/ [MMOC] SCHEME
COURANT NUMBER ALLOWED IN SOLVING THE ADVECTION TERM =   l.00
MAXIMUM  NUMBER  OF  MOVING  PARTICLES  ALLOWED  =     75000
        300000  ELEMENTS OF THE    X ARRAY USED BY THE    ADV  PACKAGE
           9760 ELEMENTS OF THE    IX ARRAY USED BY THE    ADV  PACKAGE

DSP1  --   DISPERSION  PACKAGE,   VER  1.0,  AUGUST 1990,    INPUT READ FROM UNIT 3
        97612  ELEMENTS OF THE   X   ARRAY USED BY THE DSP  PACKAGE
               0  ELEMENTS OF THE   IX ARRAY USED BY THE DSP  PACKAGE

SSM1 --SINK & SOURCE MIXING PACKAGE,  VER 1.1  AUGUST 1990, INPUT READ FROM UNIT  4
MAJOR STRESS COMPONENTS PRESENT IN THE FLOW MODEL:
        1       WELL
        2       RECHARGE
MAXIMUM  NUMBER OF POINT  SINKS/SOURCES    =     2000
        16880  ELEMENTS OF  THE    X ARRAY USED BY THE  SSM PACKAGE
          2440  ELEMENTS OF THE    IX ARRAY BY THE SSM PACKAGE

RCT1 -- CHEMICAL REACTIONS PACKAGE, VER 1.0,  AUGUST 1990, INPUT READ FROM UNIT 9
TYP E OF SORPTION SELECTED IS   [LINEAR]
NO FIRST-ORDER RATE REACTION IS SIMULATED
            12  ELEMENTS OF THE     X  ARRAY USED BY THE RCT PACKAGE
              0  ELEMENTS OF THE    IX  ARRAY USED BY THE RCT PACKAGE
............................................................
531826 ELEMENTS OF THE     X ARRAY USED OUT OF       800000
  21964 ELEMENTS OF THE    IX ARRAY USED OUT OF         80000
............................................................
LAYER NUMBER     AQUIFER TYPE
-----------------------     ----------------------
      1                1
      2                0
      3                0
      4                0
```

```
                        WIDTH ALONG ROWS (DELR) READ ON UNIT    1 USING FREE FORMAT
                        ----------------------------------------------------------------------------------------------------
        1       2     3     4       5       6     7     8     9      10      11      12      13      14      15      16      17      18      19      20
       21      22    23    24      25      26    27    28    29      30      31      32      33      34      35      36      37      38      39      40
  ........................................................................................................................................................................
 1  2000.  1600.  800.  400.   200.   100.   50.   50.   50.    50.     50.     50.     50.     50.     50.     50.     50.     50.     50.     50.
      50.     50.   50.   50.     50.     50.   50.   50.   50.    50.     50.     50.     50.     50.   100.   200.   400.   800.  1600.  2000.

  WIDTH ALONG COLS (DELC) READ ON UNIT     1  USING FREE FORMAT
  ----------------------------------------------------------------------------------------------------
        1       2     3     4       5       6     7     8     9      10      11      12      13      14      15      16      17      18      19      20
       21      22    23    24      25      26    27    28    29      30      31      32      33      34      35      36      37      38      39      40
       41      42    43    44      45      46    47    48    49      50      51      52      53      54      55      56      57      58      59      60
       61
  ......................................................................................................................................................
 1  2000.   2000.2000.1600.    800.   400.  200.  100.   50.    50.     50.     50.     50.     50.     50.     50.     50.     50.     50.     50.
      50.     50.   50.   50.     50.     50.   50.   50.   50.    50.     50.     50.     50.     50.     50.     50.     50.     50.     50.     50.
      50.     50.   50.   50.     50.     50.   50.   50.   50.    50.     50.     50.     50.   100.   200.   400.   800.  1600.  2000.  2000.
   2000.
                              TOP  ELEV. OF 1ST LAYER       =      780.0000
                              CELL THICKNESS  (DZ)          =      25.00000          FOR LAYER     1
                              CELL THICKNESS  (DZ)          =      25.00000          FOR LAYER     2
                              CELL THICKNESS  (DZ)          =      25.00000          FOR LAYER     3
                              CELL THICKNESS  (DZ)          =      25.00000          FOR LAYER     4
                              EFFECTIVE POROSITY            =    0.3000000           FOR LAYER     1
                              EFFECTIVE POROSITY            =    0.3000000           FOR LAYER     2
                              EFFECTIVE POROSITY            =    0.3000000           FOR LAYER     3
                              EFFECTIVE POROSITY            =    0.3000000           FOR LAYER     4
                              CONCN. BOUNDARY ARRAY=                          1  FOR LAYER     1
                              CONCN. BOUNDARY ARRAY=                          1  FOR LAYER     2
                              CONCN. BOUNDARY ARRAY=                          1  FOR LAYER     3
                              CONCN. BOUNDARY ARRAY=                          1  FOR LAYER     4
                              INITIAL CONCENTRATION         =    0.0000000           FOR LAYER     1

 INITIAL CONCENTRATION        FOR  LAYER   2   READ ON UNIT 99 USING FORMAT:    "(20F8.3)      "
 ------------------------------------------------------------------------------------------------------------------------------------
 INITIAL CONCENTRATION        FOR LAYER    3  READ ON UNIT 99 USING FORMAT:    "(20F8.3)      "
 ------------------------------------------------------------------------------------------------------------------------------------
                 INITIAL CONCENTRATION                        =    0.0000000           FOR LAYER 4

 VALUE INDICATING INACTIVE CONCENTRATION CELLS =         -999.9900

 OUPUT CONTROL OPTIONS
 ----------------------
 PRINT CELL CONCENTRATION USING FORMAT CODE:            8
 PRINT PARTICLE NUMBER IN EACH CELL USING FORMAT CODE:    2
 PRINT RETRDATION  FACTOR USING FORMAT CODE:        0
 DO NOT PRINT DISPERSION  COEFFICIENT
 SAVE CONCENTRATION IN UNFORMATED FILE [MT3D.UCN] ON UNIT   18

 NUMBER OF TIMES AT WHICH SIMULATION RESULT ARE SAVED =       1
 TOTAL ELAPSED TIMES AT WHICH SIMULATION RESULTS ARE SAVED:
    500.00
```

```
NUMBER OF OBSERVATION POINTS =     8
CONCENTRATION AT OBSERVATION POINTS SAVED IN FILE [MT3D.OBS] ON UNIT 17
LOCATION OF OBSERVATION POINTS
.....................................................................
NUMBER   LAYER    ROW     COLUMN
     1        3      11        29
     2        3      19        26
     3        3      26        23
     4        3      33        20
     5        3      40        17
     6        3      48        14
     7        3      48         9
     8        3      52        17

A ONE-LINE SUMMRY OF MASS BALANCE FOR EACH STEP SAVED IN FILE [MT3D.MAS] ON UNIT 19

MAXIMUM  LENGTH ALONG THE    X   (J)  AXIS   =   11600.00
MAXIMUM  LENGTH ALONG THE    Y   (I)  AXIS   =   20450.00
MAXIMUM  LENGTH ALONG THE    Z   (K)  AXIS   =   100.0000

ADVECTION SOLUTION OPTIONS
-----------------------------------------------

METHOD FOR PARTICLE TRACKING IS [MIXED ORDER]
CONCENTRATION WEIGHTING FACTOR       =          0.5 00
THE CONCENTRATION GRADIIENT CONSIDERED NEGLIGIBLE  [DCEPS]  =    0.1000000E-04
INITIAL PARTICLES ARE PLACED RANDOMLY WITHIN CELL BLOCK
PARTICLE NUMBER PER CELL IF DCCELL =< DCEPS      =    0
PARTICLE NUMBER PER CELL IF DCCELL     > DCEPS   =    10
MINIMUM PARTICLE NUMBER ALLOWD PER CELL         =    2
MAXIMUM PARTICLE NUMBER ALLOWD PER CELL         =    30
MULTIPLIER OF PARTICLE NUMBER AT SOURCE         =    1.00
SCHEME FOR CONCENTRATION INTERPOLATION IS [LINEAR]
PARTICLES FOR APPROXIMATING A SINK CELL IN THE [MMOC] SCHEME
ARE PLACED RANDOMLY WITHIN CELL BLOCK
NUMBER OF PARTICLES USED TO APPROXIMATE A SINK CELL IN THE [MMOC] SCHEME =     8
CRITICAL CONCENTRATION GRADIENT USED IN THE "HMOC" SCHEME [DCHMOC]= 0.1000E-01
THE "MOC"      SOLUTION IS USED WHEN DCCELL   >   DCHMOC
THE "MMOC"  SOLUTION IS USED WHEN DCCELL   =<   DCHMOC


DISPERSION PARAMETERS
--------------------------------------

                                LONG. DISPERSIVITY (AL)      =     10.00000    FOR LAYER   1
                                LONG. DISPERSIVITY (AL)      =     10.00000    FOR LAYER   2
                                LONG. DISPERSIVITY (AL)      =     110.00000   FOR LAYER   3
                                LONG. DISPERSIVITY (AL)      =     110.00000   FOR LAYER   1
                                H. TRANS./LONG. DISP         =     0.2000000
                                V. TRANS./LONG. DISP         =     0.2000000
                                DIFFUSION  COEFFICIENT       =     0.0000000

SORPTION AND 1ST ORDER RATE REACTION PARAMETERS
-----------------------------------------------------------------------------------

                                BULK DENSITY (RHOB)          =     0.3000000
                                SORPTION CONSTANT NO.1       =      1.000000
                                SORPTION CONSTANT NO.2       =      1.000000
```

```
                                                  STRESS PERIOD NO. 001

LENGTH OF CURRENT STRESS PERIOD     =         1000.000
NUMBER OF TIME STEPS FOR CURRENT STRESS PERIOD    =                1
TIME STEP MULTIPLIER      =     1.000000
USER-SPECIFIEDTRANSPORT STEPSIZE     =         0.0000000   DAY
MAXIMUM NUMBER OF TRANSPORT STEP ALLOWED IN ONE TIME STEP =              1000

CONCENTRATION OF RECHARGE FLUXES WILL BE READ IN STRESS PERIOD           1
                                           CONC. OF RECH. FLUX         =                  0.0000000
NO. OF POINT SINKS/SOURCES OF SPECIFIED CONCONCENTRATIONS =                  0 IN STRESS PERIOD   1


                               --------------------------
                               TIME STEP NO. 001
                               --------------------------
FROM TIME                   =    0.00000            To       1000.0

            "HEAD          " FLOW TERMS FOR TIME STEP 1, STRESS PERIOD     1 READ UNFORMATTED ON UNIT       10
            -----------------------------------------------------------------------------------------------------
            "QXX           " FLOW TERMS FOR TIME STEP 1, STRESS PERIOD     1 READ UNFORMATTED ON UNIT       10
            -----------------------------------------------------------------------------------------------------
            "QYY           " FLOW TERMS FOR TIME STEP 1, STRESS PERIOD     1 READ UNFORMATTED ON UNIT       10
            -----------------------------------------------------------------------------------------------------
            "QZZ           " FLOW TERMS FOR TIME STEP 1, STRESS PERIOD     1 READ UNFORMATTED ON UNIT       10
            -----------------------------------------------------------------------------------------------------

MAXIMUM STEPSIZE DURING WHICH ANY PARTICLE CANNOT MOVE MORE THAN ONE CELL
 =  4.822       (WHEN MIN.  R.R. = 1)    AT K=   3, I=   10,  J=   29

            "CNH           " FLOW TERMS FOR TIME STEP 1, STRESS PERIOD     1 READ UNFORMATTED ON UNIT       10
            -----------------------------------------------------------------------------------------------------
            "WEL           " FLOW TERMS FOR TIME STEP 1, STRESS PERIOD     1 READ UNFORMATTED ON UNIT       10
            -----------------------------------------------------------------------------------------------------
            "RCH           " FLOW TERMS FOR TIME STEP 1, STRESS PERIOD     1 READ UNFORMATTED ON UNIT       10
            -----------------------------------------------------------------------------------------------------

TOTAL NUMBER OF POINT SOtJRCES/SINKS PRESENT IN THE FLOW MODEL =   800


MAXIMUM  STEPSIZE WHICH MEETS STABILITY CRITERION OF THE SINK & SOURCE TERM
=  558.2       ( WHEN MIN. R.F.= 1)   AT   K  =       4,     I =       1,       J =       7

MAXIMUM STEPSIZE WHICH MEETS STABILITY CRITERION OF THE DISPERSION TERM
=  3.959        (WHEN MIN.  R.F.=l)    AT   K   =       3,     I =      48,      J =      14


--------------------------------------------
TRANSPORT STEP No.        64
--------------------------------------------
TOTAL ELAPSED TIME SINCE BEGINNING OF SIMULATION = 500.0000 DAY
 ....................................................................
            CONCENTRATIONS IN LAYER 1 AT END OF TRANSPORT STEP 64, TIME STEP 1, STRESS PERIOD 1
            ------------------------------- --------------------------------------------------------
            CONCENTRATIONS IN LAYER 2 AT END OF TRANSPORT STEP 64, TIME STEP 1, STRESS PERIOD 1
            -------------- -- ----- - -- --- -- --------- ---- -----------------------------------
            CONCENTRATIONS IN LAYER 3 AT END OF TRANSPORT STEP 64, TIME STEP 1, STRESS PERIOD 1
            -------------------------------------------------------------------------------------------
            CONCENTRATIONS IN LAYER 4 AT END OF TRANSPORT STEP 64, TIME STEP 1, STRESS PERIOD 1
            -------------------------------------------------------------------------------------------
```

```
TOTAL PARTICLES USED IN THE CURRENT STEP         57046
PA TICLE S ADDED AT BEGINNING OF THE STEP          480
PARTICLES REMOVED AT END OF LAST STEP              484

             PARTICLE NUMBER IN LAYER 1 AT END OF TRANSPORT STEP 64, TIME STEP 1, STRESS PERIOD 1
             ------------------------------------------------------------------------------------------
             PARTICLE NUMBER IN LAYER 2 AT END OF TRANSPORT STEP 64, TIME STEP 1, STRESS PERIOD 1
             ------------------------------------------------------------------------------------------
             P ARTICLE NUMBER IN LAYER 3 AT END OF TRANSPORT STEP 64, TIME STEP 1, STRESS PERIOD 1
             ------------------------------------------------------------------------------------------
             P ARTICLE NUMBER IN LAYER 4 AT END OF TRANSPORT STEP 64, TIME STEP 1, STRESS PERIOD 1
             ------------------------------------------------------------------------------------------

             CUM LATIVE MASS BUDGETS AT END OF TRANSPORT STEP 64, TIME STEP 1, STRESS PERIOD 1
             ------------------------------------------------------------------------------------------

                                          IN                 OUT
                                    ----------------      ----------------
 CONSTANT CONCENTRATION:      0.0000000              0.0000000
               CONSTANT HEAD:      0.0000000             -1731.714
                            WELLS:      0.0000000             -0.2304379E +10
                     RECHARGE :      0.0000000              0.0000000
DECAY OR BIODEGRADATION:      0.0000000              0.0000000
     MASS STORAGE (SOLUTE):      0.2539149E+10        -0.1470597E+10
   MASS STORAGE (ADSORBED)      0.2539149E+10        -0.1470597E +10
                                        -----------------------------------------------------------------------------
                                  [TOTAL]:     0.5078298E+10 UNDF  -0.5245574E+10 UNDF

                                              NET ( IN - OUT):          -0.1672760E+09
                                  DISCREPANCY (PERCENT):          -3.240568

                                                              ------------------------------------------
                                                                 TRANSPORT STEP NO. 128
                                                              ------------------------------------------

TOTAL ELAPSED TIME SINC 13EGINNING OF SIM L TION = 1000.000 DAY
 .....................................................................
             CONCENTRATIONS IN LAYER 1 AT END OF TRANSPORT STEP 128, TIME STEP 1, STRESS PERIOD 1
             ------------------------------------------------------------------------------------------
             CONCENTRATIONS IN LAYER 2 AT END OF TRANSPORT STEP 128, TIME STEP 1, STRESS PERIOD 1
             ------------------------------------------------------------------------------------------
             CONCENTRATIONS IN LAYER 3 AT END OF TRANSPORT STEP 128, TIME STEP 1, STRES PERIOD 1
             ------------------------------------------------------------------------------------------

         1      2      3      4      5      6      7      8      9     10     11     12     13     14     15     16     17     18     19     20
        21     22     23     24     25     26     27     28     29     30     31     32     33     34     35     36     37     38     39     40
      ............................................................................................................................
 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
 2     0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0   0. 0    0.0    0.0    0.0
       0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0   0.0
 3     0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
       0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
 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
       0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
 5     0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
       0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
 6     0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.1    0.1    0.1    0.1    0.1    0.1    0.1
       0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.2    0.2    0.2    0.2    0.2    0.2    0.0    0.0    0.0
 7     0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.2    0.1    0.2    0.2    0.1
       0.1    0.1    0.1    0.2    0.1    0.1    0.1    0.1    0.2    0.3    0.4    0.5    0.4    0.4    0.5    0.2    0.2    0.0    0.0    0.0
 8     0.0    0.0    0.0    0.0    0.0    0.0    0.1    0.1    0.1    0.1    0.1    0.2    0.2    0.3    0.3    0.3    0.4    0.4    0.3    0.3
       0.2    0.3    0.3    0.3    0.3    0.2    0.2    0.4    0.5    0.7    0.6    0.7    0.6    0.6    0.6    0.6    0.2    0.0    0.0    0.0
```

| | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 9 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.1 | 0.2 | 0.2 | 0.2 | 0.3 | 0.3 | 0.4 | 0.4 | 0.4 | 0.5 | 0.5 | 0.5 | 0.6 |
| | 0.4 | 0.4 | 0.4 | 0.4 | 0.3 | 0.3 | 0.4 | 0.5 | 0.6 | 0.8 | 1.0 | 0.9 | 0.8 | 0.6 | 0.7 | 0.7 | 0.3 | 0.0 | 0.0 | 0.0 |
| 10 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.1 | 0.2 | 0.2 | 0.3 | 0.4 | 0.5 | 0.5 | 0.5 | 0.7 | 0.6 | 0.8 | 0.6 | 0.8 |
| | 0.6 | 0.6 | 0.6 | 0.5 | 0.5 | 0.5 | 0.4 | 0.6 | 0.7 | 1.1 | 1.1 | 1.2 | 1.1 | 0.9 | 0.8 | 0.8 | 0.4 | 0.0 | 0.0 | 0.0 |
| 11 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.1 | 0.2 | 0.2 | 0.3 | 0.4 | 0.4 | 0.6 | 0.6 | 0.7 | 0.8 | 0.8 | 0.8 | 0.8 | 0.9 |
| | 0.7 | 0.8 | 0.8 | 0.8 | 0.6 | 0.7 | 0.7 | 0.9 | 1.1 | 1.2 | 1.5 | 1.2 | 1.3 | 1.2 | 1.1 | 1.0 | 0.5 | 0.0 | 0.0 | 0.0 |
| 12 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.1 | 0.2 | 0.3 | 0.4 | 0.4 | 0.6 | 0.7 | 0.8 | 0.9 | 1.3 | 1.3 | 1.1 | 1.1 | 1.2 |
| | 1.0 | 1.2 | 1.0 | 1.0 | 0.9 | 1.3 | 1.1 | 0.8 | 1.5 | 2.1 | 1.7 | 1.3 | 1.5 | 1.4 | 1.2 | 1.1 | 0.5 | 0.0 | 0.0 | 0.0 |
| 13 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.2 | 0.3 | 0.4 | 0.4 | 0.6 | 0.8 | 0.9 | 1.0 | 1.2 | 1.5 | 1.4 | 1.4 | 1.5 | 1.5 |
| | 1.4 | 1.4 | 1.4 | 1.3 | 1.3 | 1.5 | 1.4 | 1.9 | 2.5 | 2.7 | 2.2 | 1.9 | 1.8 | 1.6 | 1.5 | 1.3 | 0.6 | 0.0 | 0.0 | 0.0 |
| 14 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.3 | 0.4 | 0.5 | 0.6 | 0.8 | 1.0 | 1.1 | 1.3 | 1.5 | 1.7 | 1.7 | 1.8 | 2.4 | 1.8 |
| | 1.7 | 1.7 | 1.7 | 1.8 | 1.8 | 2.4 | 2.4 | 2.8 | 2.7 | 3.1 | 2.9 | 2.4 | 2.1 | 1.9 | 1.8 | 1.8 | 0.6 | 0.0 | 0.0 | 0.0 |
| 15 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.2 | 0.4 | 0.5 | 0.7 | 0.8 | 1.0 | 1.1 | 1.4 | 1.6 | 1.9 | 2.2 | 2.1 | 2.2 | 2.3 | 2.3 |
| | 2.2 | 2.9 | 2.3 | 2.5 | 2.5 | 2.8 | 3.9 | 4.2 | 3.8 | 3.6 | 3.0 | 2.7 | 2.5 | 2.2 | 1.9 | 1.5 | 0.6 | 0.0 | 0.0 | 0.0 |
| 16 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.3 | 0.5 | 0.6 | 1.0 | 0.9 | 1.2 | 1.4 | 1.7 | 1.8 | 2.2 | 2.8 | 2.6 | 2.6 | 2.8 | 2.6 |
| | 2.8 | 2.8 | 2.9 | 3.0 | 2.9 | 4.1 | 5.2 | 5.1 | 5.0 | 4.7 | 3.5 | 3.3 | 2.7 | 2.7 | 2.1 | 1.5 | 0.7 | 0.0 | 0.0 | 0.0 |
| 17 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.3 | 0.6 | 0.8 | 1.0 | 1.3 | 1.5 | 1.7 | 2.1 | 2.3 | 2.6 | 3.1 | 3.2 | 3.1 | 3.4 | 4.0 |
| | 3.7 | 3.3 | 3.4 | 3.8 | 3.5 | 4.1 | 6.5 | 5.5 | 6.0 | 4.7 | 4.6 | 3.8 | 3.4 | 2.8 | 2.6 | 1.9 | 0.7 | 0.0 | 0.0 | 0.0 |
| 18 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.4 | 0.7 | 1.0 | 1.2 | 1.5 | 1.8 | 2.2 | 2.5 | 2.8 | 3.2 | 3.5 | 3.8 | 3.7 | 4.0 | 4.2 |
| | 4.0 | 5.0 | 4.2 | 4.5 | 4.4 | 5.2 | 6.4 | 6.1 | 5.8 | 5.2 | 4.9 | 4.3 | 3.6 | 3.5 | 2.7 | 1.9 | 0.8 | 0.0 | 0.0 | 0.0 |
| 19 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.5 | 0.9 | 1.2 | 1.5 | 2.0 | 2.2 | 2.5 | 3.0 | 3.4 | 3.8 | 4.0 | 4.4 | 4.6 | 4.8 | 5.0 |
| | 4.9 | 5.1 | 5.2 | 4.5 | 4.4 | 6.8 | 8.1 | 6.4 | 6.5 | 5.9 | 5.1 | 4.4 | 4.2 | 3.3 | 2.9 | 2.0 | 0.7 | 0.0 | 0.0 | 0.0 |
| 20 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.6 | 1.0 | 1.4 | 1.7 | 2.2 | 2.7 | 3.0 | 3.5 | 4.2 | 4.8 | 4.5 | 5.2 | 5.4 | 5.8 | 5.8 |
| | 6.2 | 5.8 | 6.6 | 5.8 | 5.2 | 7.6 | 7.9 | 7.6 | 6.8 | 6.3 | 5.2 | 4.6 | 4.1 | 3.8 | 3.4 | 2.0 | 0.6 | 0.0 | 0.0 | 0.0 |
| 21 | 0.0 | 0.0 | 0.0 | 0.0 | 0.2 | 0.7 | 1.3 | 1.7 | 2.2 | 2.6 | 3.3 | 3.6 | 3.7 | 4.7 | 5.0 | 5.8 | 6.3 | 6.4 | 6.7 | 6.5 |
| | 6.9 | 6.8 | 7.9 | 6.3 | 11.7 | 9.3 | 8.9 | 8.0 | 7.3 | 6.8 | 5.8 | 5.0 | 4.5 | 4.2 | 3.6 | 1.9 | 0.7 | 0.0 | 0.0 | 0.0 |
| 22 | 0.0 | 0.0 | 0.0 | 0.0 | 0.2 | 0.9 | 1.5 | 2.0 | 2.5 | 3.0 | 3.5 | 4.2 | 5.0 | 6.7 | 6.0 | 6.5 | 6.5 | 7.5 | 7.6 | 8.2 |
| | 7.8 | 8.2 | 7.1 | 9.0 | 11.7 | 10.9 | 10.0 | 8.6 | 7.7 | 7.0 | 6.1 | 5.4 | 4.6 | 4.1 | 3.8 | 2.1 | 0.7 | 0.0 | 0.0 | 0.0 |
| 23 | 0.0 | 0.0 | 0.0 | 0.0 | 0.3 | 1.1 | 1.8 | 2.2 | 2.9 | 3.5 | 4.2 | 5.1 | 5.5 | 6.4 | 6.5 | 7.1 | 7.7 | 8.3 | 8.8 | 9.3 |
| | 8.5 | 9.5 | 9.5 | 11.4 | 13.5 | 11.5 | 10.3 | 9.0 | 8.1 | 7.2 | 6.5 | 5.6 | 4.8 | 4.4 | 3.9 | 2.1 | 0.6 | 0.0 | 0.0 | 0.0 |
| 24 | 0.0 | 0.0 | 0.0 | 0.0 | 0.4 | 1.3 | 2.1 | 2.7 | 3.3 | 4.1 | 4.6 | 5.7 | 6.4 | 7.2 | 8.0 | 8.8 | 8.4 | 9.6 | 10.0 | 10.3 |
| | 11.0 | 11.2 | 11.1 | 12.3 | 12.3 | 11.4 | 11.7 | 9.5 | 8.4 | 7.6 | 6.8 | 6.1 | 5.2 | 4.6 | 3.7 | 2.5 | 0.6 | 0.0 | 0.0 | 0.0 |
| 25 | 0.0 | 0.0 | 0.0 | 0.0 | 0.4 | 1.5 | 2.5 | 3.2 | 3.9 | 4.6 | 6.0 | 6.4 | 7.1 | 8.6 | 8.4 | 10.3 | 11.1 | 10.7 | 11.6 | 11.3 |
| | 11.4 | 11.5 | 12.0 | 16.3 | 13.5 | 13.1 | 10.5 | 9.9 | 8.8 | 7.9 | 7.2 | 6.2 | 5.2 | 5.1 | 4.3 | 2.0 | 0.6 | 0.0 | 0.0 | 0.0 |
| 26 | 0.0 | 0.0 | 0.0 | 0.0 | 0.5 | 1.8 | 2.8 | 3.6 | 4.2 | 5.7 | 6.1 | 7.2 | 8.5 | 9.0 | 9.9 | 11.0 | 11.9 | 12.2 | 13.0 | 13.2 |
| | 13.6 | 14.2 | 13.0 | 14.5 | 13.2 | 12.4 | 11.5 | 9.9 | 8.9 | 8.3 | 7.3 | 6.4 | 5.6 | 4.8 | 4.1 | 2.5 | 0.6 | 0.0 | 0.0 | 0.0 |
| 27 | 0.0 | 0.0 | 0.0 | 0.1 | 0.6 | 2.1 | 3.0 | 3.8 | 5.4 | 6.1 | 7.6 | 8.2 | 9.4 | 10.3 | 11.1 | 12.0 | 13.2 | 13.7 | 14.6 | 15.1 |
| | 14.6 | 14.5 | 15.2 | 14.4 | 13.5 | 12.4 | 11.6 | 9.8 | 9.5 | 8.0 | 7.3 | 6.5 | 4.9 | 4.2 | 3.0 | 2.4 | 0.4 | 0.0 | 0.0 | 0.0 |
| 28 | 0.0 | 0.0 | 0.0 | 0.1 | 0.7 | 2.3 | 3.5 | 4.6 | 5.8 | 6.8 | 8.1 | 9.4 | 10.0 | 10.9 | 12.7 | 14.5 | 14.7 | 15.8 | 16.2 | 19.0 |
| | 16.6 | 18.8 | 16.5 | 14.5 | 14.2 | 12.1 | 11.6 | 9.6 | 8.7 | 7.7 | 6.8 | 6.0 | 4.5 | 4.2 | 3.3 | 1.2 | 0.1 | 0.0 | 0.0 | 0.0 |
| 29 | 0.0 | 0.0 | 0.0 | 0.1 | 0.8 | 2.7 | 4.1 | 5.4 | 6.5 | 7.7 | 9.0 | 9.8 | 11.3 | 12.6 | 14.2 | 14.7 | 16.3 | 17.4 | 17.5 | 20.8 |
| | 21.8 | 21.7 | 17.3 | 14.5 | 13.3 | 12.9 | 10.7 | 9.8 | 8.6 | 7.2 | 6.2 | 5.3 | 4.7 | 3.5 | 2.6 | 1.2 | 0.3 | 0.0 | 0.0 | 0.0 |
| 30 | 0.0 | 0.0 | 0.0 | 0.1 | 0.8 | 2.6 | 4.5 | 5.4 | 7.4 | 8.5 | 10.1 | 11.2 | 12.6 | 14.4 | 15.5 | 16.9 | 20.4 | 19.0 | 20.3 | 20.5 |
| | 21.7 | 19.1 | 17.6 | 14.3 | 13.2 | 11.5 | 10.8 | 9.3 | 7.8 | 6.9 | 6.0 | 5.0 | 4.4 | 3.4 | 2.5 | 1.2 | 0.1 | 0.0 | 0.0 | 0.0 |
| 31 | 0.0 | 0.0 | 0.0 | 0.1 | 1.0 | 2.7 | 4.9 | 6.5 | 7.8 | 10.4 | 11.6 | 12.5 | 14.4 | 15.6 | 17.0 | 18.7 | 19.9 | 21.8 | 21.4 | 22.6 |
| | 22.2 | 19.8 | 15.8 | 13.9 | 12.0 | 10.8 | 9.5 | 8.3 | 7.1 | 6.2 | 5.1 | 4.8 | 3.8 | 3.1 | 2.4 | 0.8 | 0.1 | 0.0 | 0.0 | 0.0 |
| 32 | 0.0 | 0.0 | 0.0 | 0.1 | 1.1 | 2.8 | 5.5 | 7.0 | 8.9 | 9.9 | 11.3 | 13.1 | 15.3 | 17.2 | 18.2 | 19.4 | 21.3 | 21.7 | 23.3 | 22.5 |
| | 19.9 | 16.8 | 14.8 | 12.9 | 11.0 | 9.9 | 8.5 | 7.5 | 6.4 | 5.5 | 4.9 | 4.2 | 3.1 | 2.7 | 2.2 | 1.0 | 0.1 | 0.0 | 0.0 | 0.0 |
| 33 | 0.0 | 0.0 | 0.0 | 0.1 | 1.1 | 3.7 | 6.6 | 7.2 | 9.0 | 10.8 | 13.1 | 14.4 | 16.9 | 17.4 | 19.8 | 22.0 | 22.2 | 23.0 | 23.8 | 21.1 |
| | 17.5 | 15.7 | 13.9 | 12.5 | 10.7 | 9.2 | 8.0 | 6.8 | 5.7 | 4.9 | 4.2 | 3.2 | 2.5 | 2.4 | 1.5 | 0.4 | 0.1 | 0.0 | 0.0 | 0.0 |
| 34 | 0.0 | 0.0 | 0.0 | 0.1 | 1.4 | 3.5 | 5.9 | 7.7 | 9.8 | 12.0 | 13.6 | 15.3 | 16.9 | 19.4 | 20.9 | 22.4 | 23.7 | 25.3 | 25.6 | 15.9 |
| | 15.4 | 14.0 | 14.0 | 11.2 | 9.5 | 8.0 | 6.8 | 5.9 | 5.0 | 4.0 | 3.5 | 2.7 | 2.2 | 1.3 | 1.1 | 0.4 | 0.1 | 0.0 | 0.0 | 0.0 |
| 35 | 0.0 | 0.0 | 0.0 | 0.1 | 1.3 | 4.4 | 6.5 | 7.9 | 10.3 | 12.5 | 14.4 | 16.3 | 18.5 | 20.3 | 21.8 | 23.7 | 25.8 | 28.1 | 26.4 | 17.7 |
| | 14.5 | 12.7 | 11.8 | 10.3 | 8.2 | 7.1 | 6.1 | 5.1 | 4.3 | 3.5 | 2.5 | 1.6 | 1.4 | 1.2 | 0.4 | 0.3 | 0.1 | 0.0 | 0.0 | 0.0 |
| 36 | 0.0 | 0.0 | 0.0 | 0.1 | 1.6 | 4.6 | 6.3 | 8.7 | 11.1 | 12.8 | 15.0 | 17.0 | 19.2 | 21.2 | 23.2 | 25.9 | 27.4 | 28.5 | 21.4 | 15.8 |
| | 13.9 | 12.3 | 10.3 | 8.8 | 7.7 | 6.6 | 5.8 | 4.5 | 3.6 | 2.6 | 2.2 | 1.5 | 1.1 | 0.8 | 0.5 | 0.2 | 0.1 | 0.0 | 0.0 | 0.0 |
| 37 | 0.0 | 0.0 | 0.0 | 0.1 | 1.8 | 5.3 | 6.8 | 8.9 | 11.1 | 13.3 | 15.2 | 17.6 | 20.3 | 21.8 | 24.6 | 26.7 | 29.2 | 28.7 | 21.0 | 15.4 |
| | 13.2 | 11.1 | 10.0 | 7.9 | 7.0 | 5.7 | 4.7 | 3.6 | 3.0 | 2.1 | 1.6 | 1.1 | 0.7 | 0.6 | 0.4 | 0.1 | 0.1 | 0.0 | 0.0 | 0.0 |
| 38 | 0.0 | 0.0 | 0.0 | 0.1 | 1.8 | 4.2 | 7.0 | 8.4 | 10.8 | 13.3 | 16.0 | 18.2 | 21.0 | 22.8 | 24.8 | 27.2 | 29.7 | 26.6 | 17.7 | 14.5 |
| | 13.2 | 10.3 | 9.3 | 7.6 | 6.2 | 5.0 | 3.9 | 3.1 | 2.2 | 1.7 | 1.1 | 0.8 | 0.5 | 0.4 | 0.2 | 0.1 | 0.1 | 0.0 | 0.0 | 0.0 |
| 39 | 0.0 | 0.0 | 0.0 | 0.1 | 2.2 | 4.4 | 7.3 | 8.5 | 11.5 | 14.0 | 16.4 | 18.4 | 20.6 | 23.5 | 26.0 | 27.6 | 27.7 | 21.9 | 15.7 | 13.7 |
| | 12.1 | 9.7 | 8.3 | 7.1 | 5.6 | 4.5 | 3.4 | 2.4 | 1.8 | 1.4 | 1.0 | 0.6 | 0.4 | 0.3 | 0.2 | 0.1 | 0.0 | 0.0 | 0.0 | 0.0 |

```
40   0.0   0.0   0.0   0.1   2.4   3.4   7.4   8.6  11.1  13.7  16.1  18.9  20.8  22.9  25.4  24.7  23.2  16.3  14.5  12.3
    11.0   9.0   7.5   6.0   5.0   3.7   2.7   2.1   1.8   1.1   0.6   0.4   0.3   0.2   0.1   0.1   0.0   0.0   0.0   0.0
41   0.0   0.0   0.0   0.1   2.2   3.4   7.4   8.9  10.9  14.0  16.7  18.6  21.3  23.4  24.2  25.9  18.1  13.4  12.4  11.1
     9.3   7.9   7.0   5.3   4.1   3.0   2.2   1.7   1.2   0.7   0.6   0.4   0.3   0.1   0.1   0.1   0.0   0.0   0.0   0.0
42   0.0   0.0   0.0   0.1   2.2   3.6   7.2   8.4  11.5  13.7  16.1  18.8  21.8  23.3  26.1  24.0  14.3  12.0  11.0   9.8
     8.3   7.0   5.7   4.5   3.2   2.4   1.8   1.1   0.9   0.6   0.4   0.3   0.2   0.1   0.1   0.1   0.0   0.0   0.0   0.0
43   0.0   0.0   0.0   0.0   1.4   3.4   7.1   8.0  10.2  13.1  16.1  19.0  21.5  23.7  24.6  19.5  12.4  11.2   9.8   8.9
     7.3   6.3   4.8   3.7   2.6   2.0   1.4   1.1   0.7   0.5   0.3   0.2   0.1   0.1   0.1   0.0   0.0   0.0   0.0   0.0
44   0.0   0.0   0.0   0.0   1.1   3.3   4.9   7.9   9.9  12.8  15.8  18.9  21.8  24.0  24.7  15.3  12.1  10.2   8.9   7.8
     6.2   4.9   3.9   3.1   2.2   1.7   1.1   0.8   0.5   0.4   0.3   0.2   0.1   0.1   0.1   0.0   0.0   0.0   0.0   0.0
45   0.0   0.0   0.0   0.0   1.2   2.9   4.2   6.9   9.4  12.6  15.8  19.0  22.0  24.3  22.3  14.2  11.0   9.5   8.1   6.1
     5.0   4.1   3.2   2.5   1.7   1.2   0.9   0.6   0.4   0.3   0.2   0.1   0.1   0.1   0.1   0.0   0.0   0.0   0.0   0.0
46   0.0   0.0   0.0   0.0   0.9   2.6   3.1   4.6   8.3  12.1  15.5  18.5  22.1  24.0  19.1  12.6   9.9   8.0   6.5   5.2
     4.2   3.4   2.6   1.7   1.2   0.9   0.7   0.4   0.3   0.2   0.2   0.1   0.1   0.1   0.0   0.0   0.0   0.0   0.0   0.0
47   0.0   0.0   0.0   0.0   0.4   1.9   2.6   4.0   8.0  11.9  15.3  18.0  21.4  21.5  13.7  11.2   8.1   6.9   5.2   4.2
     3.0   2.4   1.9   1.5   1.1   0.6   0.5   0.3   0.2   0.2   0.1   0.1   0.1   0.1   0.0   0.0   0.0   0.0   0.0   0.0
48   0.0   0.0   0.0   0.0   0.2   1.2   1.9   2.4   6.3  11.9  15.0  16.6  16.7  14.9  10.4   8.5   7.8   5.5   4.2   3.3
     2.4   1.8   1.2   1.0   0.6   0.4   0.3   0.2   0.1   0.1   0.1   0.1   0.1   0.0   0.0   0.0   0.0   0.0   0.0   0.0
49   0.0   0.0   0.0   0.0   0.2   0.7   0.7   1.0   1.8   6.0  12.7  13.8  12.3   9.5   7.9   7.4   5.5   4.2   3.2   2.3
     1.8   1.3   0.9   0.6   0.5   0.3   0.2   0.2   0.1   0.1   0.1   0.1   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
50   0.0   0.0   0.0   0.0   0.1   0.2   0.3   0.3   0.7   1.1   3.0   4.9   5.5   6.7   7.3   6.2   4.3   3.0   2.2   1.5
     1.0   0.8   0.6   0.4   0.3   0.2   0.2   0.1   0.1   0.1   0.1   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
51   0.0   0.0   0.0   0.0   0.1   0.1   0.2   0.3   0.3   1.0   2.3   3.5   3.6   4.3   6.4   5.6   3.1   2.2   1.2   0.8
     0.6   0.5   0.3   0.3   0.2   0.2   0.1   0.1   0.1   0.1   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
52   0.0   0.0   0.0   0.0   0.1   0.1   0.1   0.2   0.3   0.9   1.8   3.9   2.7   3.0   5.1   3.1   1.7   0.9   0.6   0.5
     0.4   0.3   0.2   0.2   0.2   0.1   0.1   0.1   0.1   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
53   0.0   0.0   0.0   0.0   0.1   0.1   0.1   0.2   0.3   0.8   2.5   4.2   2.7   2.1   1.2   1.0   0.4   0.4   0.3   0.3
     0.2   0.2   0.2   0.2   0.1   0.1   0.1   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
54   0.0   0.0   0.0   0.0   0.0   0.1   0.1   0.2   0.5   1.8   3.4   3.7   3.2   0.8   0.2   0.2   0.2   0.2   0.2   0.2
     0.1   0.1   0.1   0.1   0.1   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
55   0.0   0.0   0.0   0.0   0.0   0.1   0.1   0.3   1.1   1.3   0.9   0.7   0.2   0.1   0.1   0.1   0.1   0.1   0.1   0.1
     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
56   0.0   0.0   0.0   0.0   0.0   0.1   0.1   0.2   0.3   0.2   0.2   0.2   0.2   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


57   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.1   0.1   0.1   0.1   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   0.0
58   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
     0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
59   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
     0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
60   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
     0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
61   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
     0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0


         CONCENTRATIONS  IN LAYER  4     AT END OF TRANSPORT STEP     128, TIME STEP     1, STRESS PERIOD     1
         ------------------------------------------------------------------------------------------

 TOTAL PARTICLES USED IN THE CURRENT STEP  =          56074
 PARTICLES ADDED AT BEGINNING OF THE STEP =             570
 PARTICLES REMOVED AT END OF LAST STEP       =          431

         PARTICLE NUMBER  IN LAYER  1     AT END OF TRANSPORT STEP     128, TIME STEP     1, STRESS PERIOD     1
         ------------------------------------------------------------------------------------------
         PARTICLE NUMBER  IN LAYER  2     AT END OF TRANSPORT STEP     128, TIME STEP     1, STRESS PERIOD     1
         ------------------------------------------------------------------------------------------
         PARTICLE NUMBER  IN LAYER  3     AT END OF TRANSPORT STEP     128, TIME STEP     1, STRESS PERIOD     1
         ------------------------------------------------------------------------------------------
```

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | 39 | 40 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 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 |
| 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 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 |
| 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 8 | 9 | 6 | 7 | 0 | 0 | 0 | 0 |
| 6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 3 | 7 | 5 | 4 | 12 | 11 | 10 | 7 | 0 | 9 | 9 | 9 | 7 | 3 | 10 | 6 | 4 | 7 | 3 | 3 | 3 | 6 | 7 | 3 | 0 | 0 | 0 |
| 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 8 | 9 | 10 | 7 | 4 | 8 | 7 | 7 | 12 | 6 | 11 | 5 | 8 | 4 | 7 | 9 | 13 | 8 | 6 | 6 | 8 | 8 | 4 | 12 | 5 | 9 | 11 | 0 | 0 |
| 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 10 | 9 | 5 | 5 | 7 | 6 | 11 | 10 | 9 | 6 | 8 | 9 | 8 | 5 | 15 | 7 | 3 | 5 | 10 | 6 | 6 | 14 | 9 | 5 | 6 | 10 | 7 | 6 | 7 | 4 | 3 | 0 | 0 |
| 9 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 7 | 9 | 9 | 3 | 10 | 4 | 8 | 5 | 6 | 4 | 9 | 10 | 3 | 5 | 5 | 5 | 4 | 7 | 3 | 5 | 5 | 8 | 5 | 6 | 3 | 4 | 3 | 7 | 6 | 4 | 5 | 0 | 0 |
| 10 | 0 | 0 | 0 | 0 | 0 | 0 | 12 | 8 | 7 | 5 | 6 | 10 | 10 | 12 | 11 | 10 | 3 | 7 | 10 | 11 | 8 | 5 | 9 | 4 | 6 | 11 | 5 | 5 | 13 | 6 | 8 | 15 | 8 | 4 | 7 | 4 | 6 | 6 | 0 | 0 |
| 11 | 0 | 0 | 0 | 0 | 0 | 6 | 16 | 5 | 9 | 13 | 8 | 11 | 10 | 10 | 9 | 8 | 8 | 6 | 5 | 8 | 9 | 11 | 9 | 12 | 3 | 10 | 8 | 8 | 15 | 7 | 6 | 7 | 11 | 4 | 7 | 5 | 6 | 5 | 0 | 0 |
| 12 | 0 | 0 | 0 | 0 | 0 | 12 | 11 | 6 | 6 | 8 | 10 | 5 | 7 | 7 | 11 | 6 | 9 | 11 | 9 | 8 | 6 | 14 | 5 | 11 | 13 | 7 | 5 | 6 | 16 | 10 | 9 | 5 | 12 | 4 | 4 | 6 | 11 | 9 | 0 | 0 |
| 13 | 0 | 0 | 0 | 0 | 7 | 18 | 5 | 9 | 4 | 4 | 7 | 11 | 11 | 10 | 12 | 5 | 10 | 9 | 7 | 5 | 6 | 11 | 12 | 11 | 6 | 10 | 7 | 11 | 17 | 8 | 7 | 6 | 6 | 2 | 8 | 9 | 6 | 8 | 0 | 0 |
| 14 | 0 | 0 | 0 | 0 | 15 | 9 | 7 | 13 | 11 | 4 | 11 | 10 | 5 | 6 | 10 | 9 | 9 | 10 | 6 | 8 | 13 | 12 | 5 | 12 | 12 | 9 | 10 | 15 | 9 | 10 | 11 | 12 | 5 | 5 | 7 | 3 | 5 | 10 | 0 | 0 |
| 15 | 0 | 0 | 0 | 0 | 12 | 10 | 11 | 8 | 15 | 11 | 8 | 10 | 11 | 6 | 7 | 10 | 4 | 8 | 10 | 8 | 9 | 7 | 12 | 11 | 5 | 14 | 14 | 10 | 7 | 7 | 11 | 8 | 4 | 6 | 8 | 10 | 3 | 7 | 0 | 0 |
| 16 | 0 | 0 | 0 | 0 | 4 | 16 | 6 | 10 | 6 | 4 | 6 | 9 | 4 | 11 | 9 | 5 | 9 | 14 | 9 | 8 | 7 | 13 | 13 | 11 | 11 | 8 | 12 | 12 | 6 | 7 | 12 | 11 | 7 | 7 | 8 | 10 | 7 | 3 | 0 | 0 |
| 17 | 0 | 0 | 0 | 0 | 9 | 10 | 10 | 6 | 10 | 7 | 12 | 4 | 11 | 6 | 9 | 5 | 10 | 10 | 8 | 6 | 5 | 15 | 11 | 7 | 15 | 11 | 12 | 7 | 10 | 7 | 11 | 12 | 6 | 7 | 5 | 8 | 4 | 4 | 0 | 0 |
| 18 | 0 | 0 | 0 | 7 | 10 | 18 | 10 | 10 | 11 | 10 | 12 | 13 | 7 | 9 | 5 | 13 | 15 | 6 | 9 | 9 | 12 | 10 | 9 | 10 | 8 | 13 | 9 | 9 | 3 | 8 | 5 | 6 | 8 | 3 | 7 | 8 | 10 | 9 | 0 | 0 |
| 19 | 0 | 0 | 0 | 11 | 12 | 10 | 7 | 9 | 10 | 9 | 11 | 8 | 8 | 13 | 9 | 9 | 4 | 9 | 7 | 10 | 15 | 11 | 7 | 5 | 5 | 17 | 6 | 18 | 7 | 12 | 7 | 12 | 13 | 2 | 7 | 12 | 6 | 10 | 0 | 0 |
| 20 | 0 | 0 | 0 | 13 | 11 | 20 | 9 | 11 | 13 | 6 | 6 | 7 | 6 | 12 | 7 | 6 | 4 | 5 | 12 | 12 | 12 | 5 | 8 | 10 | 8 | 5 | 9 | 9 | 7 | 6 | 5 | 16 | 9 | 10 | 7 | 5 | 7 | 5 | 0 | 0 |
| 21 | 0 | 0 | 0 | 14 | 9 | 15 | 9 | 9 | 11 | 10 | 12 | 13 | 6 | 11 | 6 | 11 | 5 | 6 | 9 | 4 | 14 | 8 | 9 | 12 | 6 | 13 | 8 | 7 | 13 | 9 | 12 | 9 | 8 | 6 | 10 | 6 | 12 | 12 | 0 | 0 |
| 22 | 0 | 0 | 0 | 13 | 13 | 20 | 12 | 8 | 10 | 9 | 9 | 11 | 9 | 4 | 8 | 11 | 6 | 6 | 13 | 12 | 3 | 7 | 8 | 11 | 11 | 13 | 6 | 11 | 11 | 9 | 7 | 8 | 6 | 12 | 10 | 7 | 5 | 6 | 0 | 0 |
| 23 | 0 | 0 | 0 | 15 | 15 | 7 | 9 | 4 | 9 | 10 | 8 | 9 | 10 | 10 | 12 | 9 | 12 | 3 | 13 | 6 | 12 | 8 | 12 | 13 | 10 | 3 | 6 | 8 | 9 | 9 | 11 | 13 | 6 | 5 | 11 | 6 | 7 | 5 | 0 | 0 |
| 24 | 0 | 0 | 0 | 11 | 13 | 14 | 13 | 6 | 14 | 9 | 9 | 5 | 13 | 11 | 13 | 9 | 3 | 10 | 14 | 6 | 16 | 10 | 9 | 9 | 9 | 5 | 8 | 7 | 7 | 3 | 9 | 12 | 8 | 5 | 5 | 9 | 13 | 9 | 0 | 0 |
| 25 | 0 | 0 | 0 | 12 | 11 | 11 | 10 | 6 | 6 | 7 | 5 | 11 | 9 | 13 | 12 | 9 | 13 | 17 | 10 | 14 | 11 | 11 | 8 | 9 | 14 | 12 | 10 | 8 | 10 | 8 | 9 | 11 | 7 | 10 | 9 | 9 | 10 | 3 | 0 | 0 |
| 26 | 0 | 0 | 0 | 12 | 13 | 10 | 9 | 9 | 10 | 9 | 8 | 10 | 11 | 12 | 5 | 11 | 11 | 8 | 14 | 9 | 12 | 6 | 17 | 7 | 7 | 12 | 12 | 10 | 12 | 6 | 9 | 7 | 5 | 6 | 3 | 5 | 6 | 7 | 0 | 0 |
| 27 | 0 | 0 | 0 | 13 | 14 | 10 | 10 | 6 | 7 | 13 | 8 | 10 | 6 | 14 | 7 | 7 | 7 | 11 | 12 | 4 | 9 | 15 | 7 | 12 | 12 | 11 | 10 | 6 | 10 | 6 | 5 | 16 | 11 | 10 | 5 | 8 | 9 | 9 | 0 | 0 |
| 28 | 0 | 0 | 0 | 11 | 15 | 7 | 11 | 8 | 5 | 10 | 13 | 12 | 8 | 13 | 12 | 14 | 14 | 13 | 10 | 9 | 13 | 13 | 17 | 10 | 11 | 9 | 13 | 5 | 8 | 10 | 9 | 12 | 8 | 11 | 9 | 4 | 8 | 6 | 0 | 0 |
| 29 | 0 | 0 | 0 | 13 | 11 | 11 | 10 | 7 | 15 | 10 | 8 | 9 | 12 | 11 | 8 | 6 | 6 | 9 | 9 | 11 | 10 | 8 | 10 | 15 | 14 | 10 | 7 | 11 | 3 | 10 | 6 | 12 | 10 | 5 | 3 | 12 | 10 | 10 | 0 | 0 |
| 30 | 0 | 0 | 0 | 13 | 6 | 13 | 9 | 10 | 14 | 12 | 11 | 10 | 15 | 16 | 8 | 13 | 9 | 10 | 8 | 17 | 14 | 15 | 7 | 14 | 13 | 12 | 4 | 14 | 8 | 10 | 8 | 7 | 9 | 8 | 9 | 5 | 8 | 3 | 0 | 0 |
| 31 | 0 | 0 | 0 | 13 | 7 | 7 | 12 | 7 | 10 | 6 | 6 | 13 | 12 | 8 | 10 | 13 | 7 | 9 | 12 | 7 | 12 | 10 | 11 | 15 | 11 | 9 | 8 | 16 | 8 | 13 | 8 | 7 | 14 | 5 | 9 | 3 | 9 | 10 | 0 | 0 |
| 32 | 0 | 0 | 0 | 7 | 10 | 11 | 9 | 14 | 10 | 14 | 11 | 6 | 12 | 11 | 8 | 10 | 8 | 8 | 8 | 4 | 12 | 8 | 11 | 12 | 6 | 5 | 7 | 7 | 14 | 7 | 14 | 9 | 5 | 6 | 12 | 4 | 8 | 0 | 0 | 0 |
| 33 | 0 | 0 | 0 | 14 | 13 | 14 | 6 | 15 | 13 | 18 | 12 | 9 | 5 | 6 | 13 | 8 | 5 | 8 | 5 | 19 | 11 | 9 | 15 | 11 | 8 | 13 | 6 | 10 | 12 | 13 | 7 | 9 | 6 | 5 | 6 | 4 | 7 | 0 | 0 | 0 |
| 34 | 0 | 0 | 0 | 13 | 8 | 9 | 9 | 9 | 9 | 13 | 8 | 14 | 10 | 9 | 7 | 8 | 7 | 12 | 6 | 6 | 6 | 9 | 11 | 6 | 12 | 12 | 8 | 11 | 11 | 11 | 10 | 9 | 8 | 5 | 8 | 8 | 11 | 0 | 0 | 0 |
| 35 | 0 | 0 | 0 | 6 | 10 | 9 | 12 | 9 | 12 | 7 | 16 | 8 | 12 | 11 | 7 | 10 | 9 | 13 | 18 | 10 | 9 | 10 | 9 | 11 | 6 | 10 | 8 | 6 | 7 | 9 | 10 | 9 | 6 | 3 | 13 | 4 | 9 | 0 | 0 | 0 |
| 36 | 0 | 0 | 0 | 14 | 10 | 7 | 7 | 9 | 7 | 6 | 10 | 11 | 8 | 5 | 12 | 13 | 11 | 6 | 16 | 9 | 8 | 9 | 8 | 10 | 11 | 6 | 8 | 7 | 6 | 10 | 8 | 9 | 12 | 6 | 5 | 14 | 10 | 0 | 0 | 0 |
| 37 | 0 | 0 | 0 | 8 | 12 | 6 | 4 | 10 | 16 | 12 | 5 | 13 | 11 | 7 | 17 | 11 | 15 | 10 | 9 | 5 | 7 | 7 | 13 | 11 | 11 | 17 | 5 | 13 | 9 | 12 | 12 | 9 | 10 | 12 | 4 | 11 | 0 | 0 | 0 | 0 |
| 38 | 0 | 0 | 0 | 13 | 7 | 5 | 8 | 7 | 8 | 9 | 12 | 9 | 11 | 11 | 17 | 10 | 14 | 13 | 15 | 6 | 7 | 9 | 11 | 8 | 15 | 10 | 6 | 13 | 5 | 13 | 9 | 8 | 3 | 6 | 11 | 4 | 0 | 0 | 0 | 0 |
| 39 | 0 | 0 | 0 | 7 | 10 | 7 | 7 | 8 | 12 | 10 | 11 | 8 | 11 | 10 | 7 | 9 | 10 | 13 | 9 | 6 | 8 | 4 | 11 | 7 | 10 | 15 | 14 | 7 | 8 | 8 | 8 | 9 | 10 | 5 | 5 | 0 | 0 | 0 | 0 | 0 |
| 40 | 0 | 0 | 0 | 14 | 9 | 4 | 5 | 5 | 10 | 11 | 13 | 10 | 17 | 10 | 15 | 12 | 14 | 4 | 7 | 8 | 9 | 13 | 6 | 13 | 5 | 10 | 11 | 6 | 7 | 6 | 8 | 11 | 5 | 6 | 4 | 0 | 0 | 0 | 0 | 0 |
| 41 | 0 | 0 | 0 | 9 | 8 | 5 | 14 | 5 | 8 | 13 | 6 | 11 | 8 | 9 | 13 | 20 | 13 | 8 | 12 | 13 | 15 | 7 | 8 | 8 | 11 | 12 | 7 | 10 | 7 | 10 | 7 | 5 | 8 | 6 | 3 | 0 | 0 | 0 | 0 | 0 |
| 42 | 0 | 0 | 0 | 8 | 7 | 5 | 6 | 13 | 9 | 15 | 8 | 12 | 8 | 7 | 14 | 15 | 11 | 5 | 7 | 7 | 7 | 12 | 10 | 11 | 9 | 6 | 11 | 3 | 13 | 5 | 14 | 10 | 14 | 8 | 4 | 0 | 0 | 0 | 0 | 0 |
| 43 | 0 | 0 | 0 | 8 | 9 | 9 | 8 | 10 | 11 | 8 | 11 | 6 | 12 | 11 | 14 | 16 | 9 | 11 | 8 | 8 | 6 | 9 | 8 | 10 | 7 | 6 | 10 | 9 | 6 | 16 | 9 | 6 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 44 | 0 | 0 | 0 | 8 | 6 | 6 | 4 | 5 | 7 | 12 | 9 | 14 | 9 | 12 | 10 | 14 | 12 | 9 | 6 | 14 | 8 | 6 | 4 | 7 | 6 | 11 | 12 | 8 | 11 | 9 | 9 | 12 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 45 | 0 | 0 | 0 | 10 | 15 | 11 | 7 | 12 | 6 | 9 | 9 | 8 | 14 | 7 | 11 | 9 | 9 | 5 | 8 | 8 | 10 | 8 | 8 | 8 | 14 | 11 | 11 | 11 | 10 | 7 | 15 | 4 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 46 | 0 | 0 | 0 | 13 | 3 | 10 | 4 | 3 | 11 | 16 | 9 | 15 | 8 | 12 | 7 | 8 | 16 | 9 | 14 | 7 | 5 | 9 | 12 | 9 | 9 | 9 | 10 | 7 | 11 | 10 | 3 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 47 | 0 | 0 | 0 | 10 | 8 | 7 | 6 | 9 | 13 | 9 | 10 | 8 | 11 | 9 | 7 | 10 | 10 | 9 | 14 | 12 | 5 | 13 | 14 | 10 | 7 | 9 | 11 | 10 | 13 | 6 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 48 | 0 | 0 | 0 | 7 | 13 | 7 | 8 | 9 | 11 | 9 | 10 | 13 | 7 | 17 | 11 | 12 | 14 | 7 | 5 | 8 | 6 | 12 | 9 | 12 | 10 | 10 | 18 | 9 | 2 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 49 | 0 | 0 | 0 | 14 | 11 | 6 | 11 | 15 | 8 | 9 | 21 | 13 | 11 | 12 | 12 | 8 | 6 | 10 | 11 | 10 | 11 | 10 | 8 | 11 | 11 | 11 | 12 | 12 | 11 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 50 | 0 | 0 | 0 | 0 | 8 | 8 | 4 | 7 | 5 | 14 | 6 | 10 | 16 | 21 | 14 | 7 | 17 | 7 | 12 | 14 | 10 | 10 | 10 | 15 | 17 | 15 | 11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 51 | 0 | 0 | 0 | 0 | 10 | 4 | 7 | 11 | 7 | 12 | 11 | 13 | 7 | 12 | 11 | 18 | 5 | 5 | 5 | 6 | 11 | 7 | 17 | 11 | 4 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 52 | 0 | 0 | 0 | 0 | 0 | 0 | 6 | 11 | 11 | 14 | 7 | 8 | 9 | 9 | 9 | 12 | 18 | 11 | 12 | 17 | 19 | 20 | 6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 53 | 0 | 0 | 0 | 0 | 0 | 0 | 6 | 10 | 11 | 14 | 8 | 10 | 3 | 8 | 10 | 8 | 7 | 7 | 16 | 12 | 7 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 54 | 0 | 0 | 0 | 0 | 0 | 0 | 8 | 16 | 20 | 17 | 16 | 12 | 7 | 4 | 10 | 9 | 9 | 9 | 9 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 55 | 0 | 0 | 0 | 0 | 0 | 0 | 10 | 24 | 23 | 26 | 8 | 10 | 16 | 5 | 13 | 15 | 6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 56 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 23 | 10 | 12 | 11 | 15 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 57 | 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 |

```
58 0   0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
59 0   0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
60 0   0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
61 0   0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0




        PARTICLE NUMBER IN LAYER 4 AT END OF TRANSPORT STEP 128, TIME STEP 1, STRESS PERIOD  1
        ------------------------------------------------------------------------------------------
        CUMULATIVE MASS BUDGETS  AT  END OF TRANSPORT STEP 128, TIME STEP   1, STRESS PERIOD    1
        ------------------------------------------------------------------------------------------

                                                        IN                        OUT
                                                 ----------------          ----------------
                    CONSTANT CONCENTRATION:          0.0000000                 0.0000000
                             CONSTANT HEAD:          0.0000000                -15501.60
                                    WEL LS:          0.0000000                -0.3497644E+10
                                  RECHARGE:          0.0000000                 0.0000000
                   DECAY OR BIODEGRADATION:          0.0000000                 0.0000000
                    MASS STORAGE (SOLUTE):           0.3485359E+10            -0.1835388E.+10
                   MASS STORAGE (ADSORBED):          0.3485359E+10            - 0.1 835388E+10
                                           ------------------------------------------------------------------------
                                   [TOTAL]:          0.6970718E+10 UNDF       -0.7168435E+10 UNDF

                                                  NET (IN - OUT):        -0.1977170E+09
                                          DISCREPANCY (PERCENT):         -2.796730

M T
3  D      End of Model Output
```

# Appendix D

# POST-PROCESSING PROGRAMS

## Appendix D
## POST-PROCESSING PROGRAMS

*The Post-Processing Program Disk* contains two programs for use in conjunction with the MT3D model: 1) POSTMT3D for generating plot data files from the unformatted concentration file (MT3D.UCN) and the model grid configuration file (MT3D.CNF), both saved by the MT3D model; and 2) SAVELAST for extracting the concentration at the last step from the unformatted concentration file (MT3D.UCN) and saving it in a separate file as the starting concentration for a continuation run. These two programs are explained in this appendix.

### D.1 POSTMT3D

POSTMT3D can be used to extract the simulated concentrations within a user-specified window at any desired transport step from the unformatted concentration file (MT3D.UCN), and save them in such a form that they can be used by most commercially available graphic software packages to generate contour maps or other types of plots.

POSTMT3D operates on the unformatted concentration file (MT3D.UCN) and the model grid configuration file (MT3D.CNF), both of which are saved when running MT3D by setting the flag SAVUCN=T. The structures and contents of these two files are as follows:

<u>MT3D.UCN (saved unformatted):</u>

For each transport step saved:

For each layer of the three-dimensional concentration matrices:

Record 1: NTRANS,KSTP,KPER,TIME2,TEXT,NCOL,NROW,ILAY

Record 2: ((CNEW(J,I,ILAY),J=l,NCOL),I=l,NROW)

where

NTRAN

S is the number of the transport step at which the concentration is saved;

KSTP is the number of the time step at which the concentration is saved;

KPER is the number of the stress period at which the concentration is saved;

TIME2 is the total elapsed time2 at which the concentration is saved;

TEXT is a character string set equal to "CONCENTRATION";

NCOL is the total number of columns;

NROW is the total number of rows;

IIAY is the layer at which the concentration is saved; and

CNEW is the simulated concentration.

MT3D.CNF (saved in free format):

Record 1: NLAY, NROW, NLAY<br>
Record 2: (DELR(J), J=l,NCOL)<br>
Record 3: (DELC(l),I=l,NROW)<br>
Record 4: ((HTOP(J,I), J=l,NCOL),I=l,NROW)<br>
Record 5: (((DZ(J,I,K), J=l,NCOL),I=l,NROW),K=l,NLAY)<br>
Record 6: CINACT

where

NLAY is the total number of layers;<br>
DELR is the cell width along the row direction;<br>
DELC is the cell width along the column direction;<br>
HTOP is the top elevation of the first model layer,<br>
DZ is the thickness of each cell in the grid; and<br>
CINACT is the value used in the model for indicating inactive concentration cells.

POSTMT3D is an interactive program. To run it, simply type the name of its executable file. The program will prompt the user for the various input items. The user can select the concentration at the desired step by specifying either the number of the transport step, time step and stress period, or the total elapsed time, which ever is more convenient. The user can also define a "window" within which the graphic data files are desired by specifying the cell indices (column, row and layer) at the *upper left* and *lower right* corners of the window. For example, to generate a data file for a cross sectional contour map along the 5th column, from row 20 to row 40 and from layer 1 to 10, enter the (J,I,K) indices at the upper left comer as 5,20, 1, and at the lower right corner as 5,40,10. Similarly, to generate a data file for a cross sectional contour map along the 5th row, from column 20 to column 40 and from layer 1 to 10, enter the (J,I,K) indices at the upper left corner as 20,5,1, and at the lower right corner as 40, 5,10. Moreover, to generate a data file for a contour map on the 5th layer, from column 20 to column 40 and from row 1 to row 10, enter the (J,I,K) indices at the upper left corner as 20,1,5 and at the lower right corner as 40,10,5. Finally, to generate a data file for a contour map on the water table, i.e., the cells in the uppermost active layers instead of a specific layer, from column 20 to column 40 and from row 1 to row 10, enter the (J,I,K) indices at the upper left corner as 20,1,0 and at the lower right corner as 40, 10,0.

For output, POSTMT3D can write data files in two formats, referred to as the "TOPO" format and the "GRID" format, according to the convention used by Golden Software's SURFER® graphic package. The TOPO format as listed below writes the concentration within a user-defined window of *regular* model mesh spacing to an output file, directly useable for generating contour maps by a contouring program such as the TOPO program included in SURFER®. The GRID format as listed below writes the concentration at each node with the nodal coordinates within the user-defmed window to the output file. This format is useful for generating data files of *irregular* model mesh spacing to be used by a gridding program such as the GRID program included in SURFER® in order to be contoured. It is also useful for generating plots of concentration versus distance along a column, row or layer at a selected time. (Note that the plots of concentration versus time at a selected node can be generated from the observation point file, M13D.OBS, saved by NMD.)

It should be pointed out that in the MT3D model, the coordinate system is defined as shown in Fig. 4.2 in Chapter 4, i.e., the origin is set at cell (1, 1, 1) and the positive x, y and z coordinates are in the directions of increasing column, row, and layer numbers, respectively. However, in the output files generated by POSTMT3D, the origin is always set at the lower left corner of the mapping window. The transformation of coordinates is done by the POSTMT3D program automatically.

TOPO format (saved in free format):

```
DSAA
NX, NY, XMAX, YMIN, YMAX, CMIN, CMAX
((CWIN(JJ,II),JJ= 1,NX),][I=NY, 1,- 1)
```

where

DSAA is the TOPO format identifier,
NX is the number of nodal points in the horizontal direction of the window;
NY is the number of nodal points in the vertical direction of the window;
XMIN is the minimum nodal coordinate in the horizontal direction of the window;
XMAX is the maximum nodal coordinate in the horizontal direction of the window;
YMIN is the minimum nodal coordinate in the vertical direction of the window;
YMAX is the maximum nodal coordinate in the vertical direction of the window;
CMIN is the minimum concentration value within the window;
CMAX is the maximum concentration value within the window; and
CWIN is the simulated concentration within the mapping window

GRID format (saved in free format):

For each active cell:

```
X, Y, CXY
```

where

X is the nodal coordinate in the horizontal direction of the window;
Y is the nodal coordinate in the vertical direction of the window;
CXY is the simulated concentration at the node defined by (X,Y).

## D.2 SAVELAST

If a continuation run as described in Section 6.10 is desired, the concentration from the final step of the preceding run can be used as the starting concentration for the continuation run. The concentration is saved in the default unformatted concentration ffle, MT3D.UCN, which is directly readable by the array reader RARRAY. If there is more than one step of concentration saved in MT3D.UCN, then SAVEIAST can be used to extract the concentration at the final step and put it in a separate unformatted file . To run it, simply type the SAVELAST executable file name and enter the names of input and output files.

# Appendix E

# ABBREVIATED INPUT INSTRUCTIONS

## BASIC TRANSPORT PACKAGE

| ID | VARIABLE NAME | FORMAT | EXPLANATION |
|---|---|---|---|
| Al | HEADING(1) | A80 | First line of title for simulation run |
| A2 | HEADING(2) | A80 | Second line of the title |
| A3 | NLAY, NROW,NCOL,NPER | 4I10 | Number of layers, rows, columns and stress periods |
| A4 | TUNIT, LUNIT, MUNIT | 3A4 | Unit names for time, length, and mass |
| A5 | TRNOP(10) | 10L2 | Transport options (ADV, DSP, SSM, RCT) |
| A6 | LAYCON(NLAY) | 40I2 | Model layer type code |
| A7 | DELR(NCOL) | RARRAY | Cell width along rows (or x-axis) |
| A8 | DELC (NROW) | RARRAY | Cell width along columns (or y-axis) |
| A9 | HTOP (NCOL, NROW) | RARRAY | Top elevation of the first model layer |
| A10 | DZ (NCOL, NROW) (One array for each layer) | RARRAY | Cell thickness |
| A11 | PRSITY (NCOL, NROW) (One array for each layer) | RARRAY | Porosity |
| A12 | ICBUND (NCOL, NROW) (One array for each layer) | IARRAY | Concentration boundary indicator array |
| A13 | SCONC (NCOL, NROW) (One array for each layer) | RARRAY | Starting concentrations |
| A14 | CINACT | F10.0 | Value indicating inactive concentration cells |
| A15 | IFMTCN,IFMTNP,IFMTRF,IFMTDP,SAVUCN | 4I10, L10 | Output control options |
| A16 | NPRS | I10 | Interval for printing or saving simulation results |
| (Enter A17 if NPRS > 0) | | | |
| A17 | TIMPRS (NPRS) | 8F10.0 | Total elapsed times at which simulation results should be printed or saved |
| A18 | NOBS | I10 | Number of observation points |
| (Enter A19 NOBS times if NOBS > 0) | | | |
| A19 | KOBS, IOBS, JOBS | 3I10 | Location of observation points (layer, row, column) |
| A20 | CHKMAS | L10 | Flag for saving mass balance summary file |
| (Repeat A21 through A23 for each stress period) | | | |
| A21 | PERLEN, NSTP, TSMULT | F10.0, I10, F10.0 | Length of stress period, number of time steps, time step multiplier |
| (Enter A22 if TSMULT < or = 0) | | | |
| A22 | TSLNGH (NSTP) | 8F10.0 | Length of time steps if geometric progression of time steps is not used in flow model |
| A23 | DTO, MXSTRN | F10.0, I10 | Transport stepsize, maximum transport steps allowed in one time step |

**ADVECTION PACKAGE**

| ID | VARIABLE NAME | FORMAT | EXPLANATION |
|---|---|---|---|
| B1 | MIXELM, PERCEL, MXPART | I10, F10.0, I10 | Advection solution flag; number of cells that any particle is allowed to move in one transport step; maximum number of moving particles allowed<br>MIXELM = 1, MOC<br>= 2, MMOC<br>= 3, HMOC<br>= 0, Finite difference |
| (Enter B2 if MIXELM = 1, 2 or 3) | | | |
| B2 | ITRACK, WD | I10, F10 | Particle tracking option, concentration weighting factor |
| (Enter B3 if MIXELM=1 or 3) | | | |
| B3 | DCEPS,NPLANE,NPL,NPH,NPMIN, NPMAX,SRMULT | F10.0, 5I10, F10.0 | Particle distribution control parameters for the MOC scheme |
| (Enter B4 of MIXELM=2, or 3) | | | |
| B4 | INTERP, NLSINK, NPSINK | 3I10 | Solution flags for the MMOC scheme |
| (Enter B5 if MIXELM=3) | | | |
| B5 | DCHMOC | F10.0 | Critical cell concentration gradient for controlling the selective use of the MOC or MMOC scheme:<br>MOC is used if DCCELL > DCHMOC;<br>MMOC is used if DCCELL < or = DCHMOC |

**DISPERSION PACKAGE**

| ID | VARIABLE NAME | FORMAT | EXPLANATION |
|---|---|---|---|
| C1 | AL (NCOL, NROW) (One array for each layer) | RARRAY | Longitudinal dispersivity |
| C2 | TRPT (NLAY) | RARRAY | Ratio of horizontal transverse dispersivity to longitudinal dispersivity |
| C3 | TRPV (NLAY) | RARRAY | Ratio of vertical transverse dispersivity to longitudinal dispersivity |
| C4 | DMCOEF (NLAY) | RARRAY | Effective molecular diffusion coefficient |

**SINK & SOURCE MIXING PACKAGE**

| **ID** | **VARIABLE NAME** | **FORMAT** | **EXPLANATION** |
|---|---|---|---|
| D1 | FWEL, FDRN, FRCH, FEVT, FRIV, FGHB | 6L2 | Flags for well, drain, recharge, evapotranspiration, river,<br>general-head-dependent boundary, respectively |
| D2 | MXSS | I10 | Maximum number of all point sources and sinks in the flow model |
| (Repeat D3 through D8 for each stress period)<br>(Enter D3 if FRCH=T) | | | |
| D3 | INCRCH | I10 | Flag indicating whether concentration of recharge flux should be read |
| (Enter D4 if FRCH=T and INCRCH > or = 0) | | | |
| D4 | CRCH (NCOL, NROW) | RARRAY | Concentration of recharge flux |
| (Enter D5 if FEVT = T) | | | |
| D5 | INCEVT | I10 | Flag indicating whether concentration of evapotranspiration fluxes should be read |
| (Enter D6 if FEVT = T and INCEVT > or = 0) | | | |
| D6 | CEVT (NCOL, NROW) | RARRAY | Concentration of evapotranspiration flux |
| D7 | NSS | I10 | Number of point sources of specified concentrations |
| (Enter D8 NSS times if NSS > 0) | | | |
| D8 | KSS, ISS, JSS, CSS, ITYPE | 3I10, F10.0,I10 | Layer, row, column, concentration, and type of point sources which are of specific concentrations<br>ITYPE = 1, constant-head cell<br>= 2, well<br>= 3, drain<br>= 4, river<br>= 5, general-head-dependent boundary cell |

## CHEMICAL REACTION PACKAGE

| ID | VARIABLE NAME | FORMAT | EXPLANATION |
|---|---|---|---|
| El | ISOTHM, IREACT | 2I10 | Flags indicating type of sorption and first order rate reactions<br>ISOTHM =1, Linear<br>= 2, Freundlich<br>= 3, Langmuir<br>= 0, None<br>IREACT = 1, Decay or biodegradation<br>= 0, None |
| (Enter E2, E3 and E4 if ISOTHM > 0) | | | |
| E2 | RHOB (NLAY) | RARRAY | Bulk density of the porous mediuin |
| E3 | SP1 (NLAY) | RARRAY | First sorption constant |
| E4 | SP2 (NLAY) | RARRAY | Second sorption constant |
| (Enter E5 and E6 if IREACT > 0) | | | |
| E5 | RC1 (NLAY) | RARRAY | First-order rate reaction constant for the dissolved phase |
| E6 | RC2 (NLAY) | RARRAY | First-order rate reaction constant for the sorbed phase |

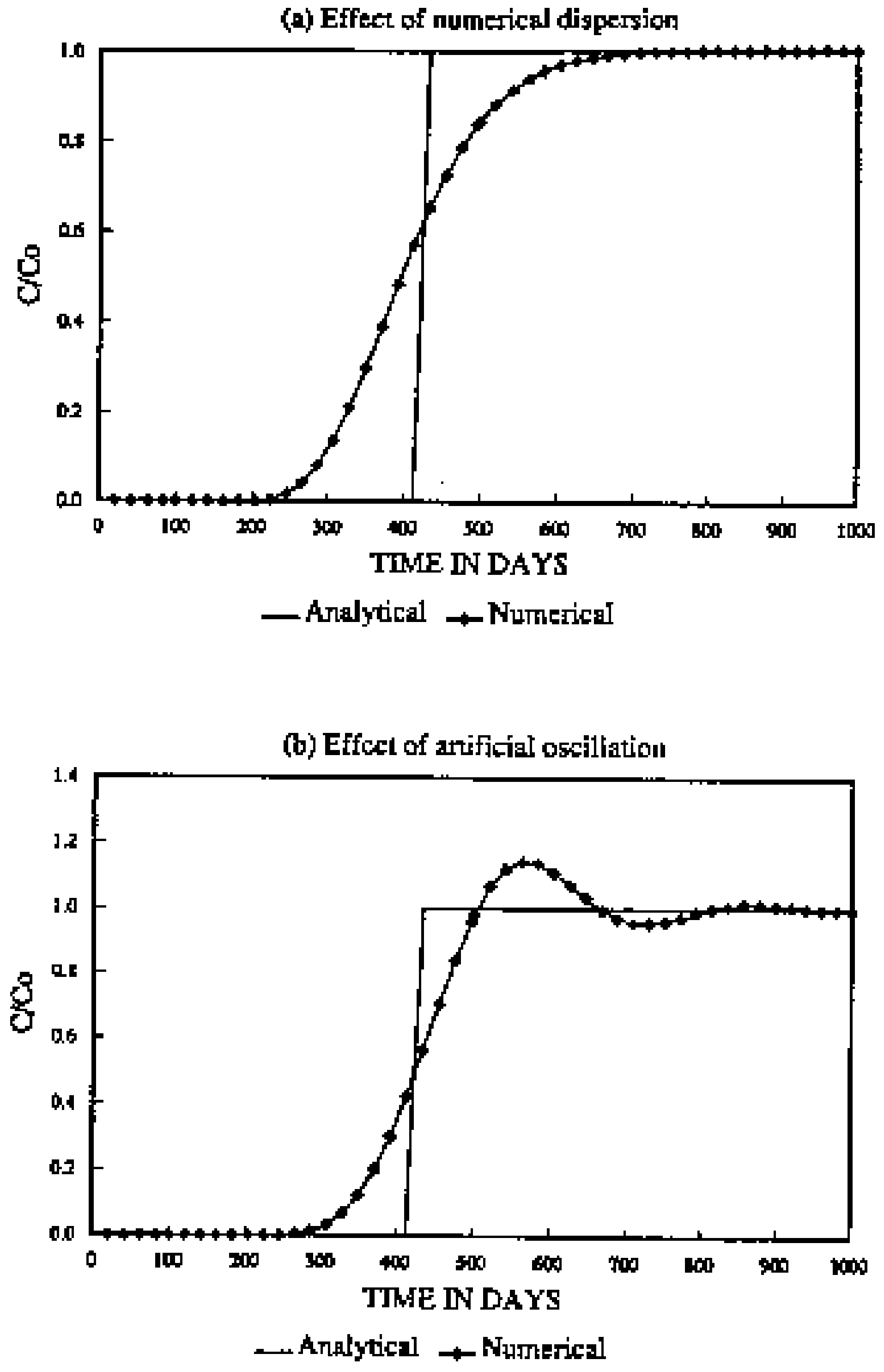


Fig. 2.1. Illustration of common numerical errors in contaminant transport modeling.

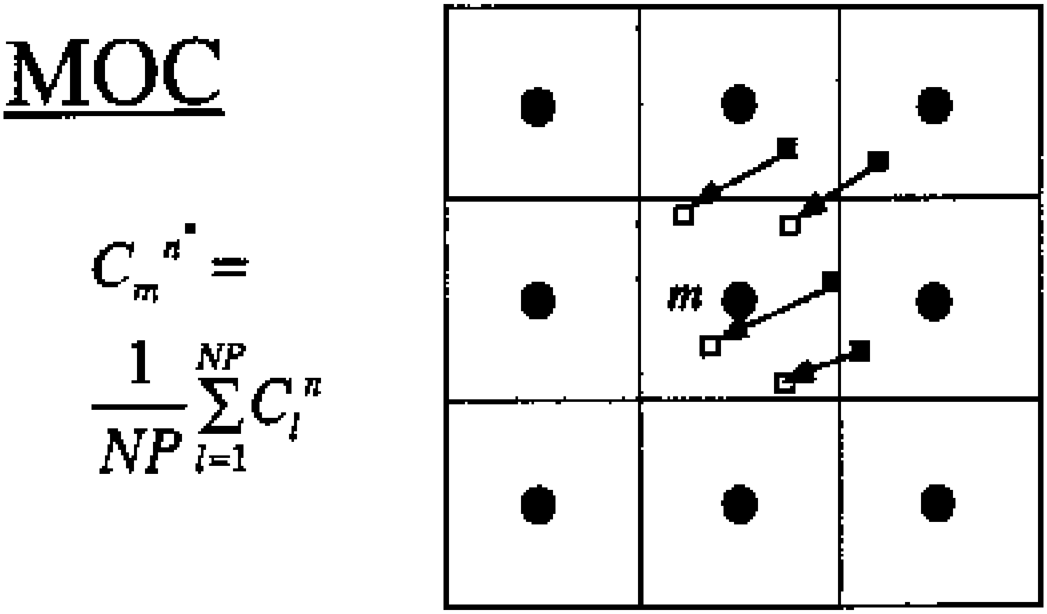


Fig. 3.1. Illustration of the Method Of Characteristics (MOC). A set of moving particles are tracked forward during each time period. An intermediate concentration, equal to the average of the concentrations of all particles in the cell, is assigned to each cell. This intermediate concentration accounts for the effect of advection during the period since the preceding time level, and is used to calculate changes in concentration due to dispersion and other processes over that period.

MMOC

$$C_m^{n^*} = C_P^{n}$$

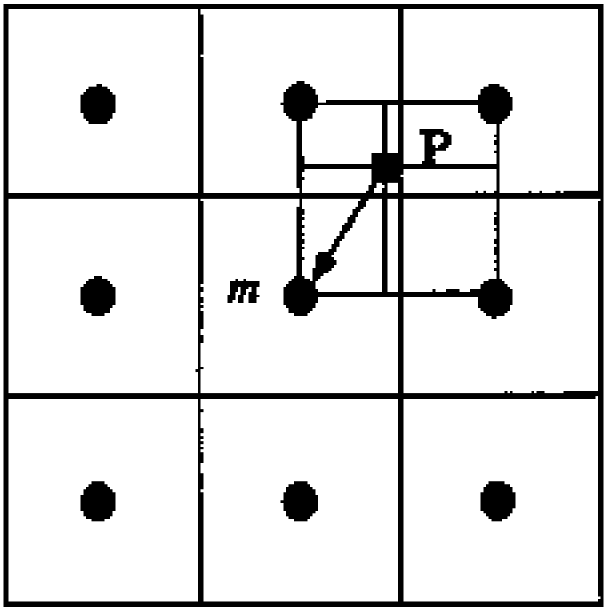


Fig. 3.1. Illustration of the Modified Method Of Characteristics (MMOC). One fictitious particle is placed at each node and tracked backward in time to find its position at the previous time level. The concentration associated with that position is the intermediate concentration due to the effect of advection during the period since the preceding time level.

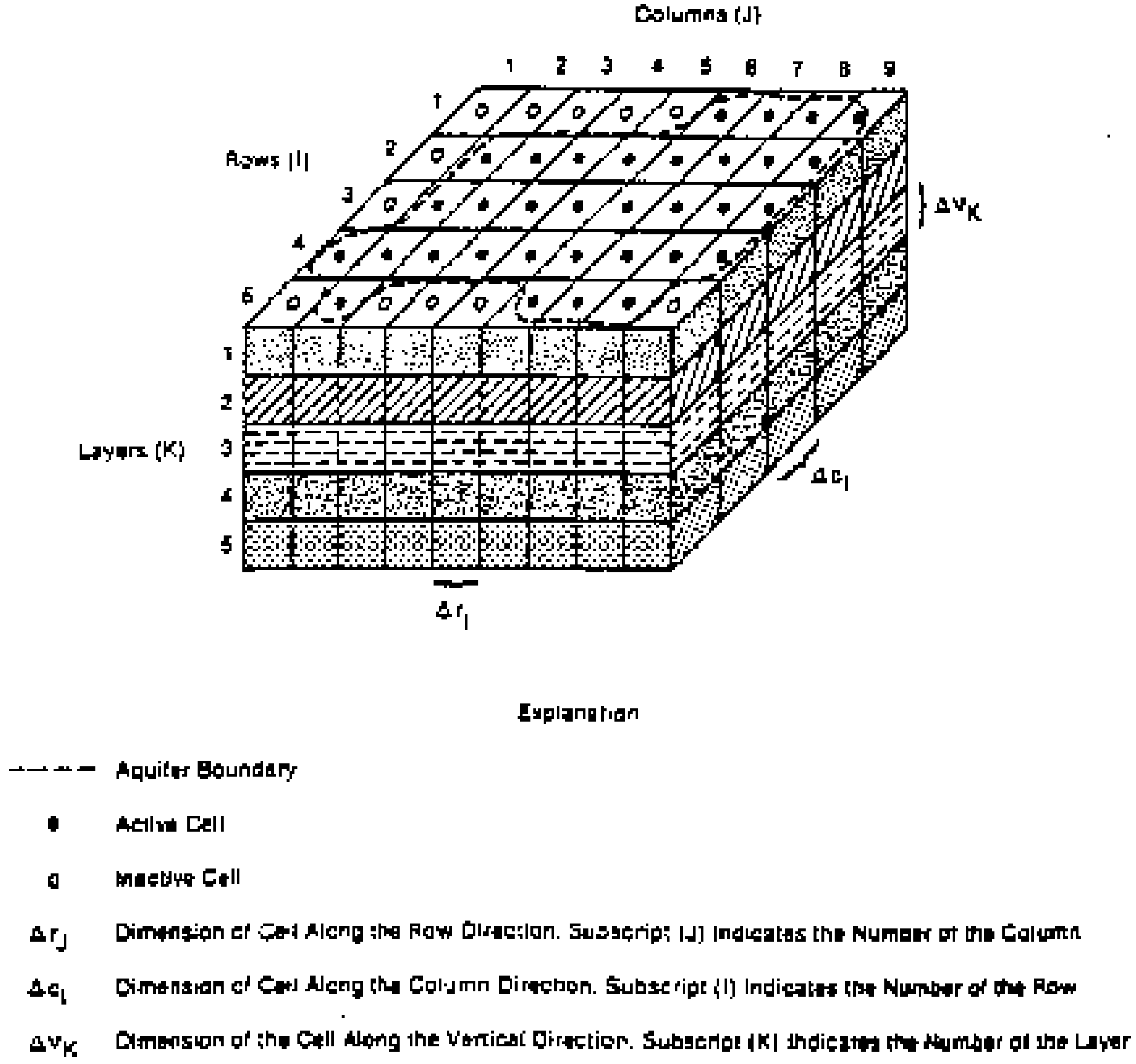
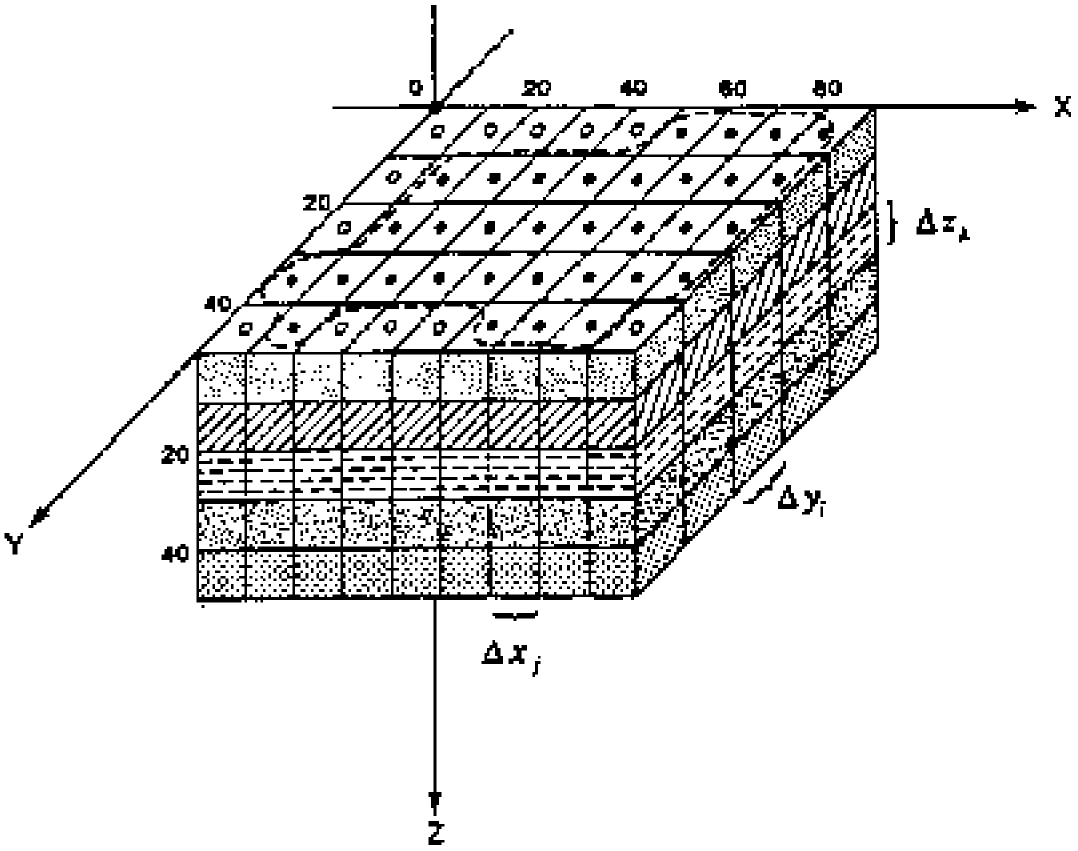

Columns (J)
1 2 3 4 5 6 7 8 9
Rows (I)
1
2
3
4
5
Layers (K)
1
2
3
4
5
ΔvK
Δci
Δrj
Explanation
Aquifer Boundary
● Active Cell
○ Inactive Cell
Δrj Dimension of Cell Along the Row Direction. Subscript (J) Indicates the Number of the Column
Δci Dimension of Cell Along the Column Direction. Subscript (I) Indicates the Number of the Row
ΔvK Dimension of the Cell Along the Vertical Direction. Subscript (K) Indicates the Number of the Layer

**Fig. 4.1.** Spatial discretization of an aquifer system (after McDonald and Harbaugh, 1988).



Assuming that:

$\Delta x_j = 10$ Along the row (x) direction

$\Delta y_i = 10$ Along the column (y) direction

$\Delta z_k = 10$ Along the layer (z) direction

Fig. 4.2. Cartesian coordinate system used in the MT3D transport model.

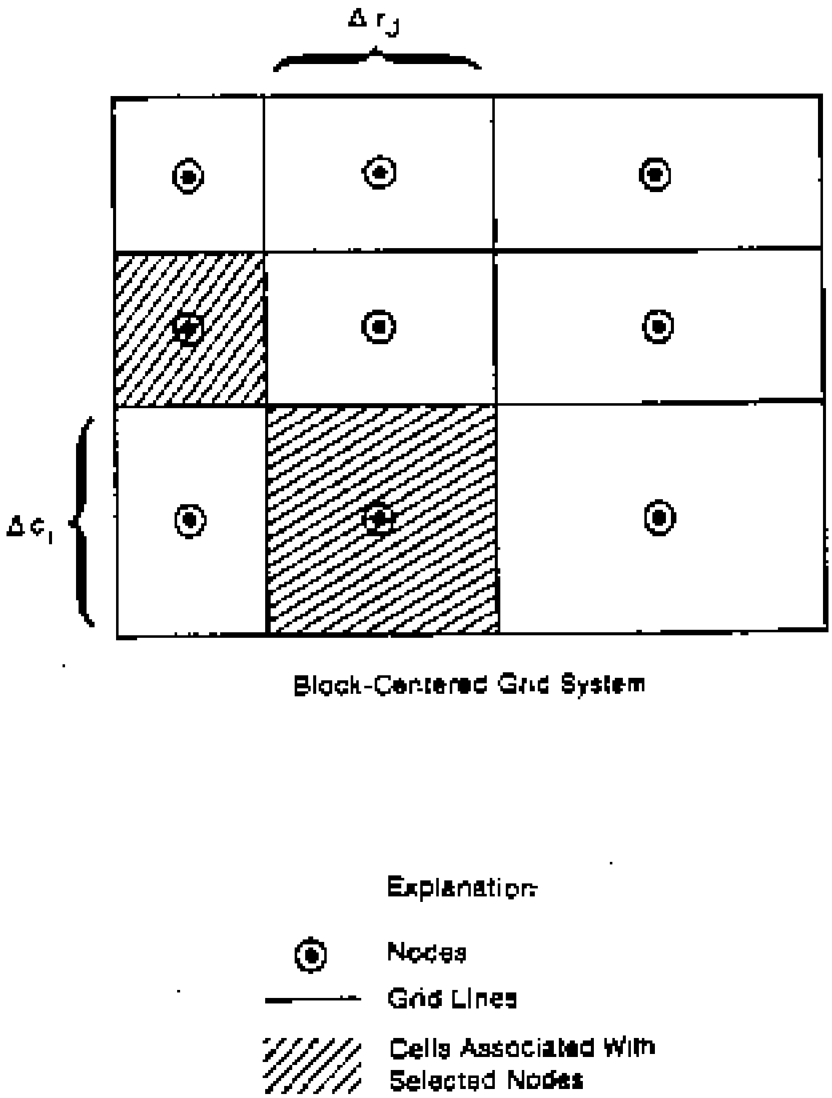

Δ r_j
Δ c_i
Block-Centered Grid System
Explanation
Nodes
Grid Lines
Cells Associated With Selected Nodes

Fig. 4.3. Diagram showing the block-centered grid system (after McDonald and Harbaugh, 1988).

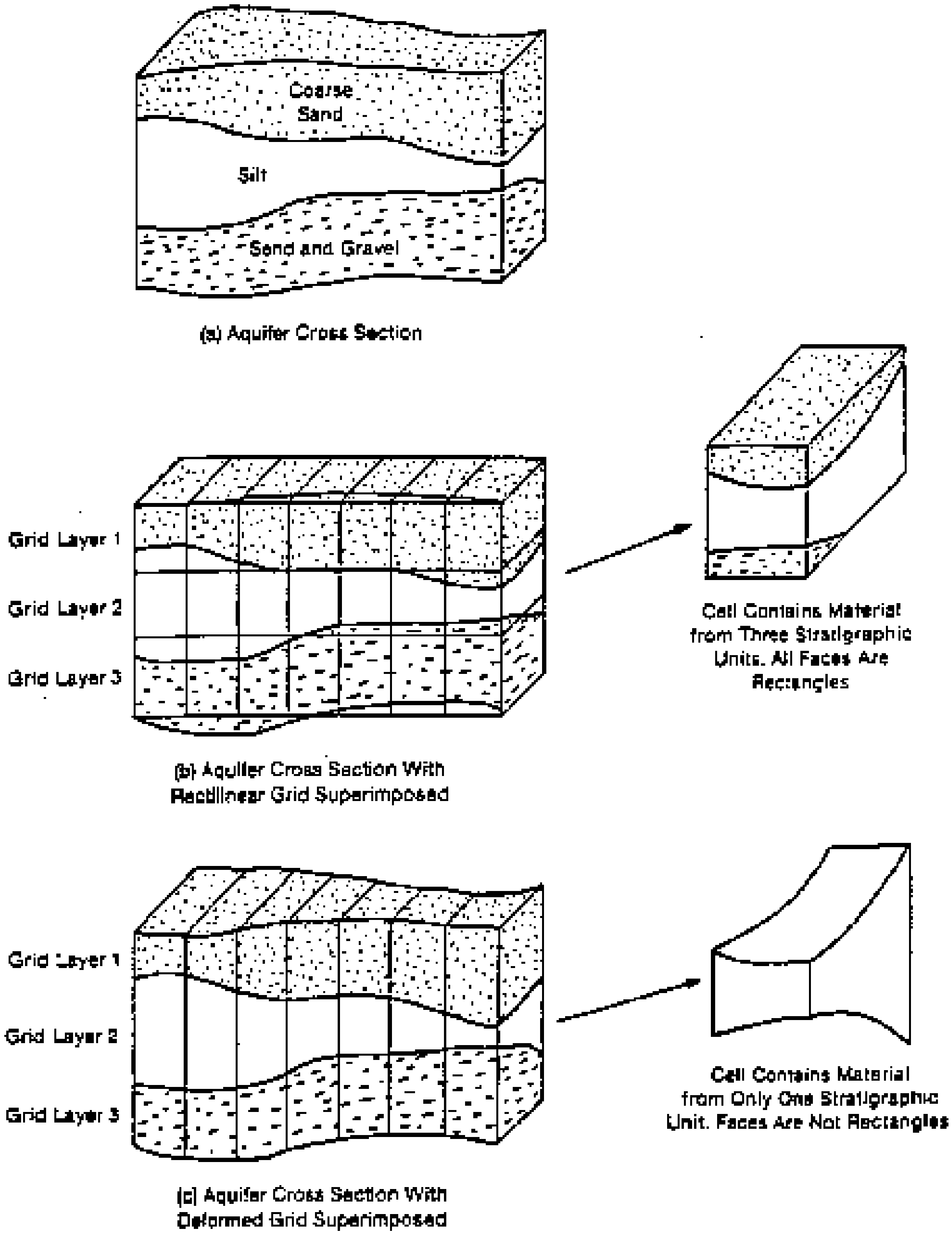
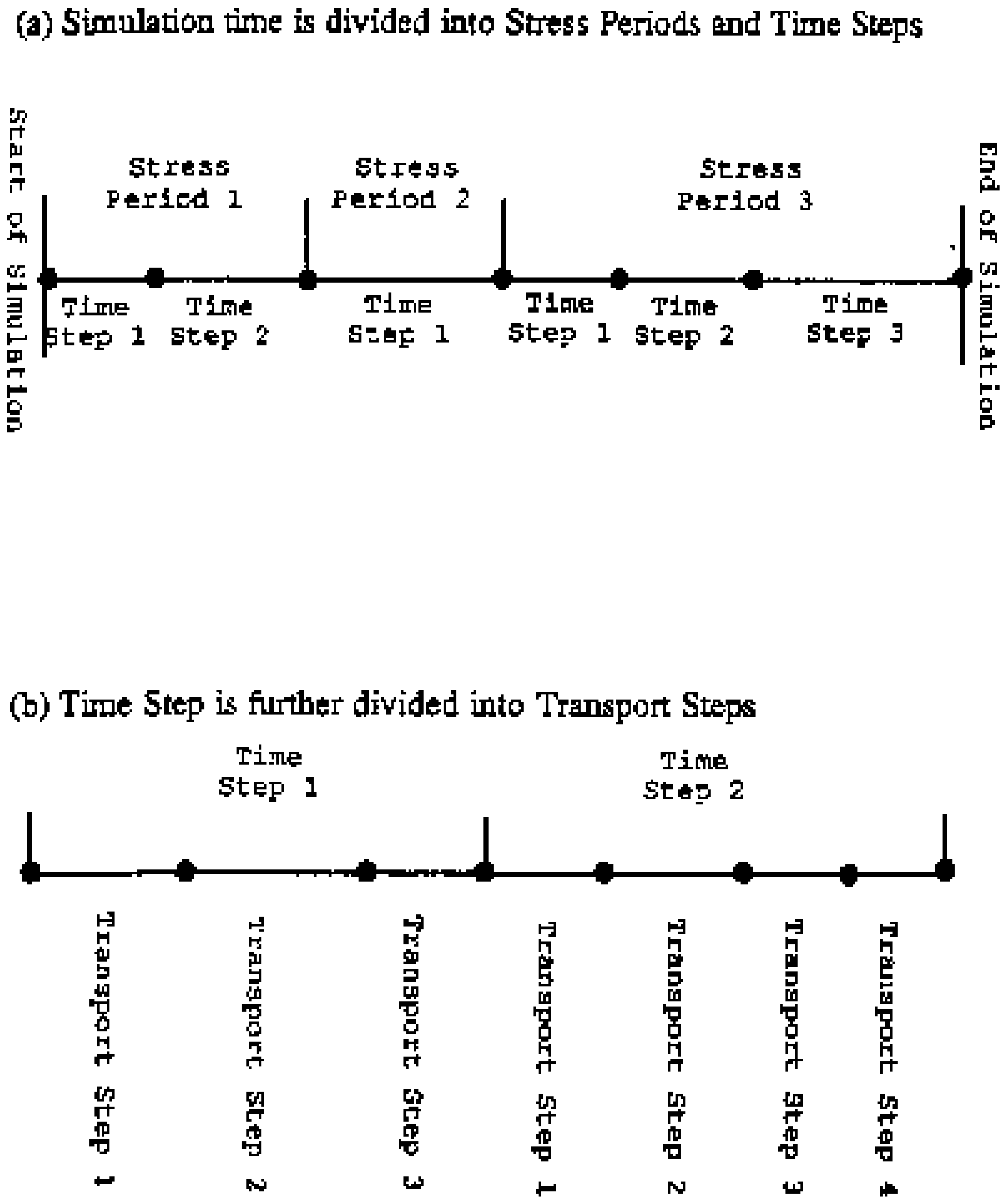

Coarse Sand
Silt
Sand and Gravel
(a) Aquifer Cross Section
Grid Layer 1
Grid Layer 2
Grid Layer 3
Cell Contains Material from Three Stratigraphic Units. All Faces Are Rectangles
(b) Aquifer Cross Section With Rectilinear Grid Superimposed
Grid Layer 1
Grid Layer 2
Grid Layer 3
Cell Contains Material from Only One Stratigraphic Unit. Faces Are Not Rectangles
(c) Aquifer Cross Section With Deformed Grid Superimposed

Fig. 4.4. Schemes of vertical discretization (after McDonald and Harbaugh, 1988).



(a) Simulation time is divided into Stress Periods and Time Steps

(b) Time Step is further divided into Transport Steps

Fig. 4.5. Discretization of simulation time in the transport model.

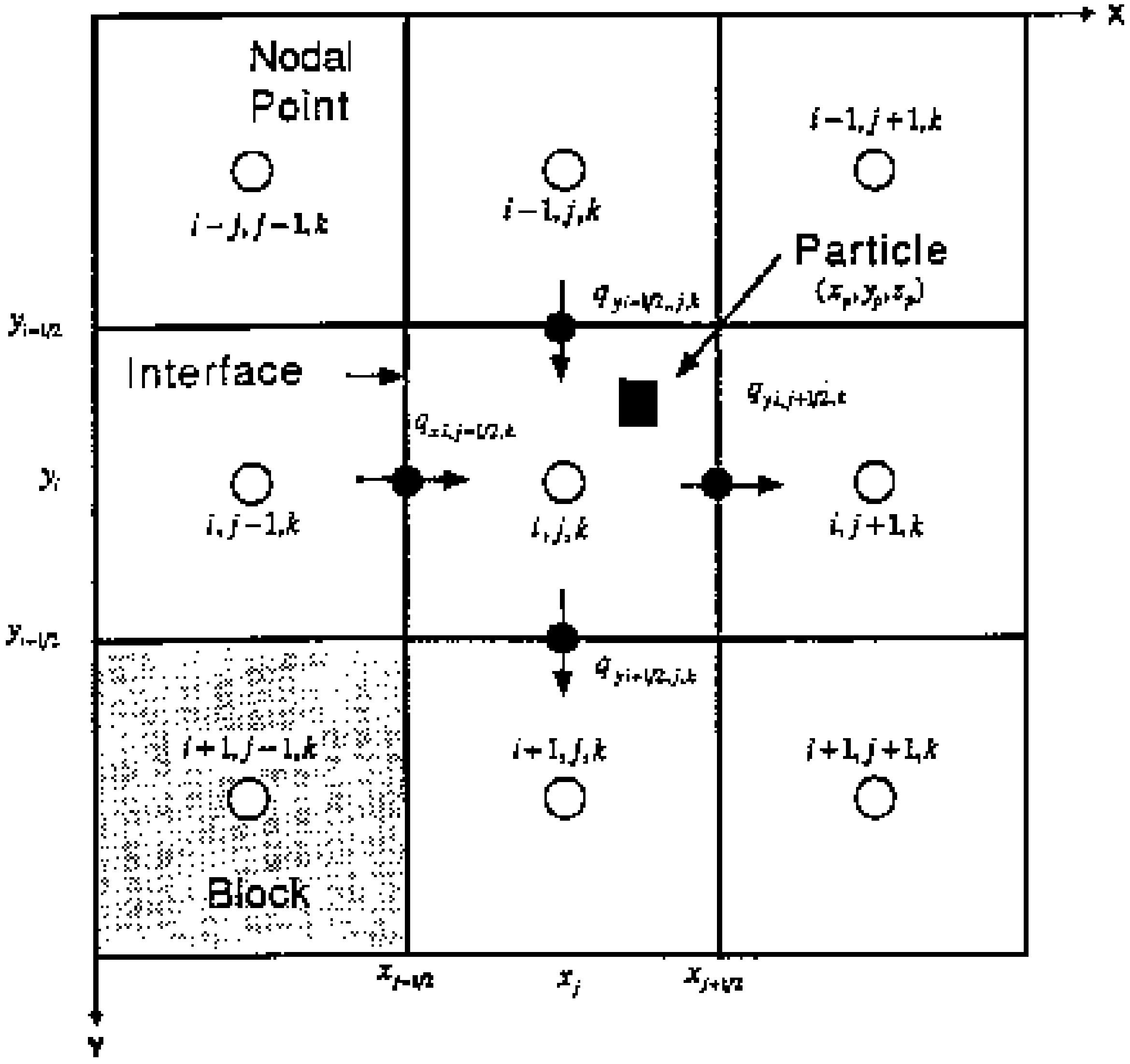


Fig. 4.6. The velocity interpolation scheme used in particle tracking.

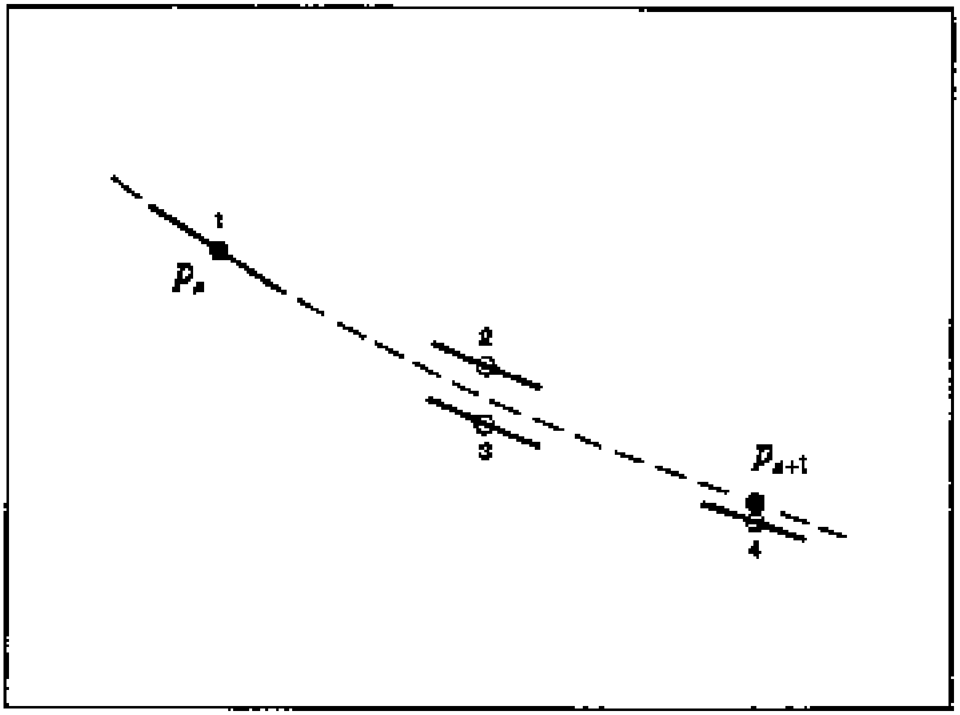
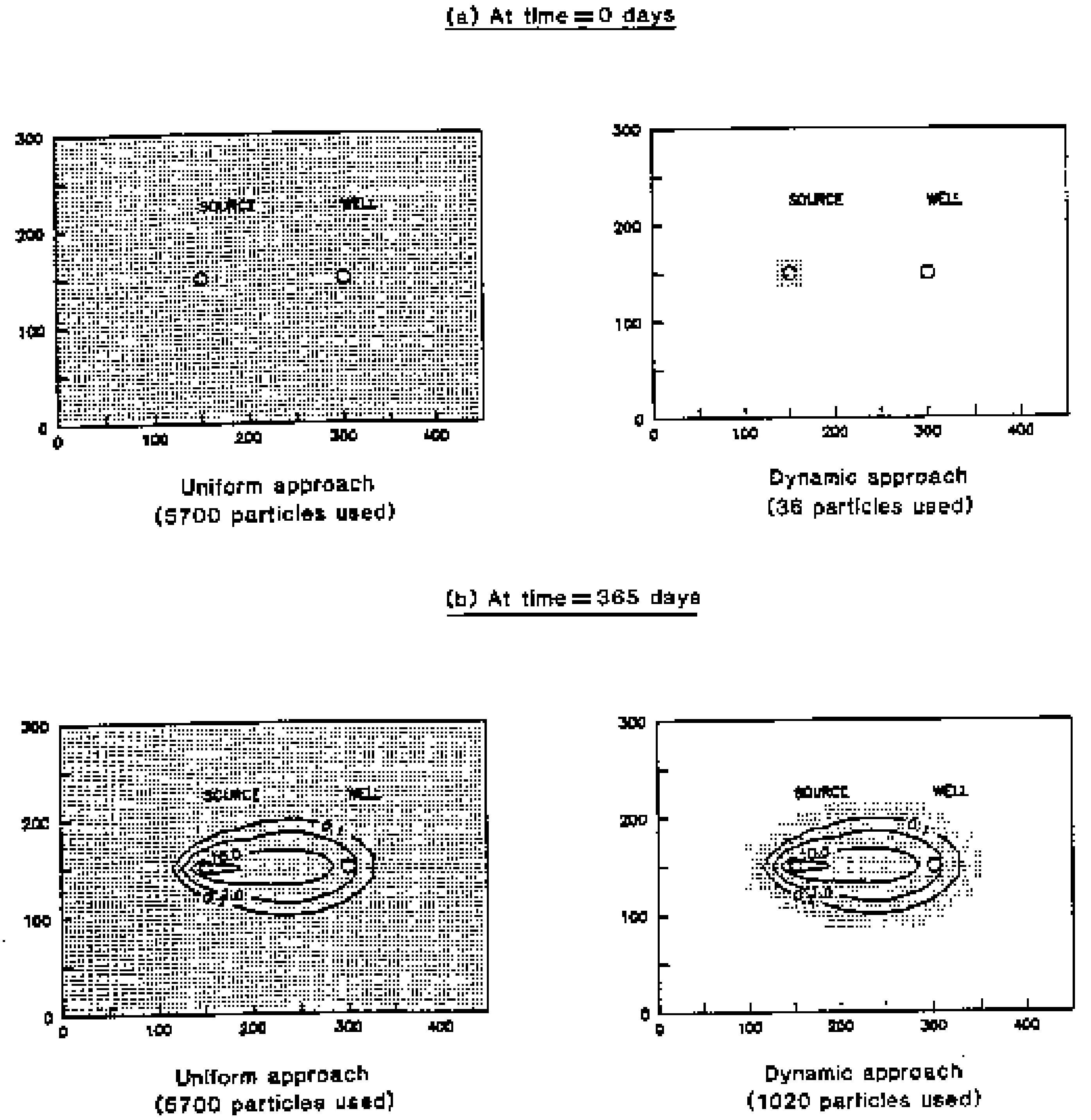


Fig. 4.7. The fourth-order Runge-Kutta method. In each step, the velocity is evaluated four times: once at the initial point, twice at trial midpoints, and once at a trial endpoint. From these velocities a weighted velocity is calculated which is used to compute the final position of the particle (shown as a filled dot). (Modified from Press et. al., 1986).



(a) At time = 0 days

Uniform approach
(5700 particles used)

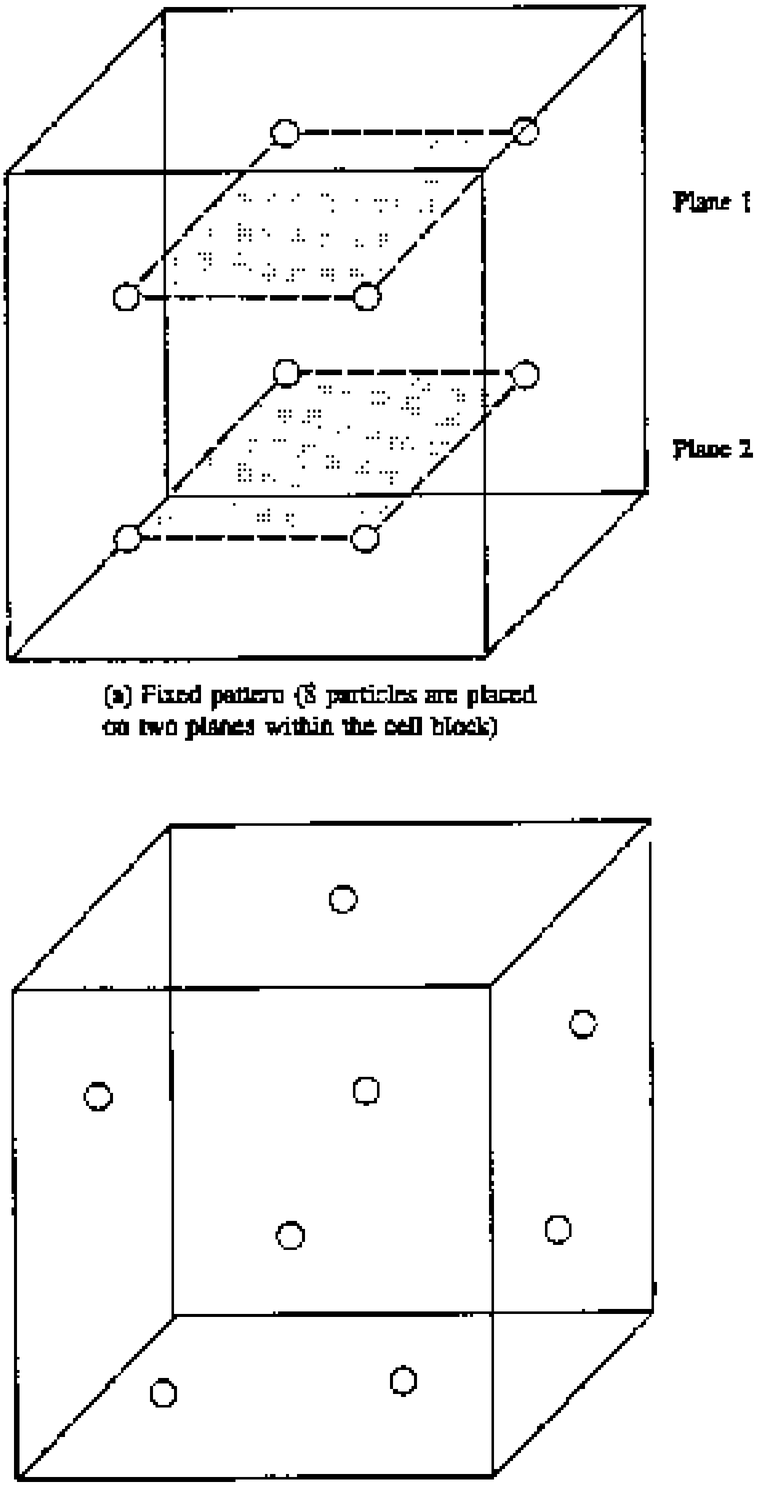
Dynamic approach
(36 particles used)

(b) At time = 365 days

Uniform approach
(6700 particles used)

Dynamic approach
(1020 particles used)

Fig. 4.8. Comparison of the uniform and dynamic approaches in controlling the distribution of moving particles.



(a) Fixed pattern (8 particles are placed on two planes within the cell block)

(b) Random pattern (8 particles are placed randomly within the cell block)

Fig. 4.9. Initial placement of moving particles.

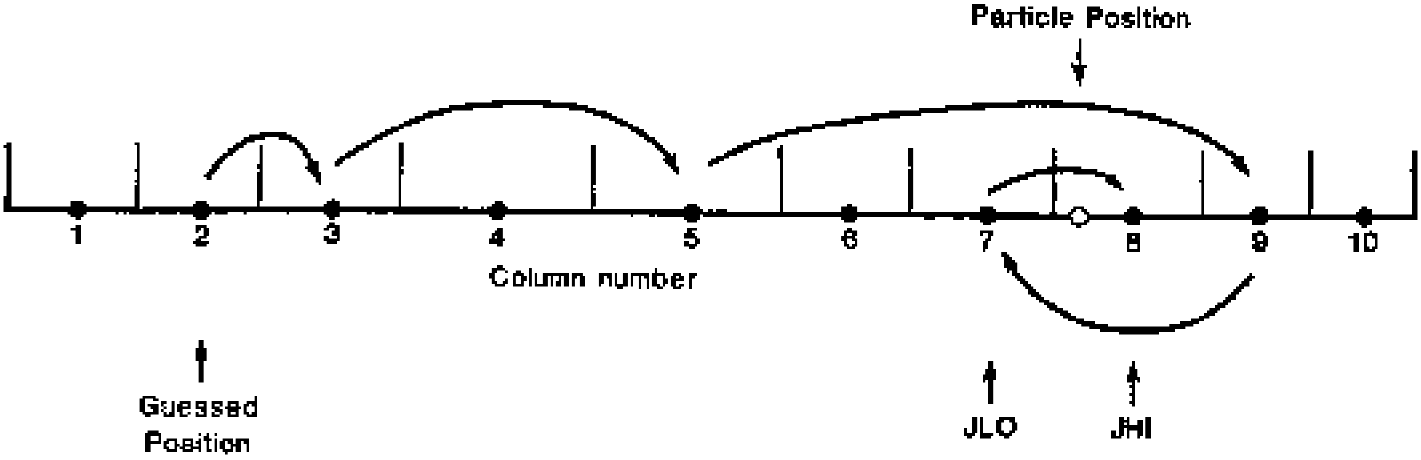


**Fig. 4.10.** To determine in which cell a particle P is located in an irregular mesh, a searching procedure is first started from a guessed position, either up or down, in increments of one, two, then four, etc., until the desired value is bracketed. Second, a bisection routine is used to bisect the nodal points in the immediate vicinity of the particle position, JLO and JHI. Finally, the coordinate of the particle is compared with that of the interface between JLO and JHI to find out whether P is locate in cell JLO or cell JHI. In this example, if the guessed position were J = 7 instead of J = 2, the cell index of P would have been located in far fewer steps. In the particle tracking calculations, the next particle to be moved is usually adjacent to the particle that has just been moved; thus the cell indices of the particle just moved are used as the guessed indices for the particle to be moved next.

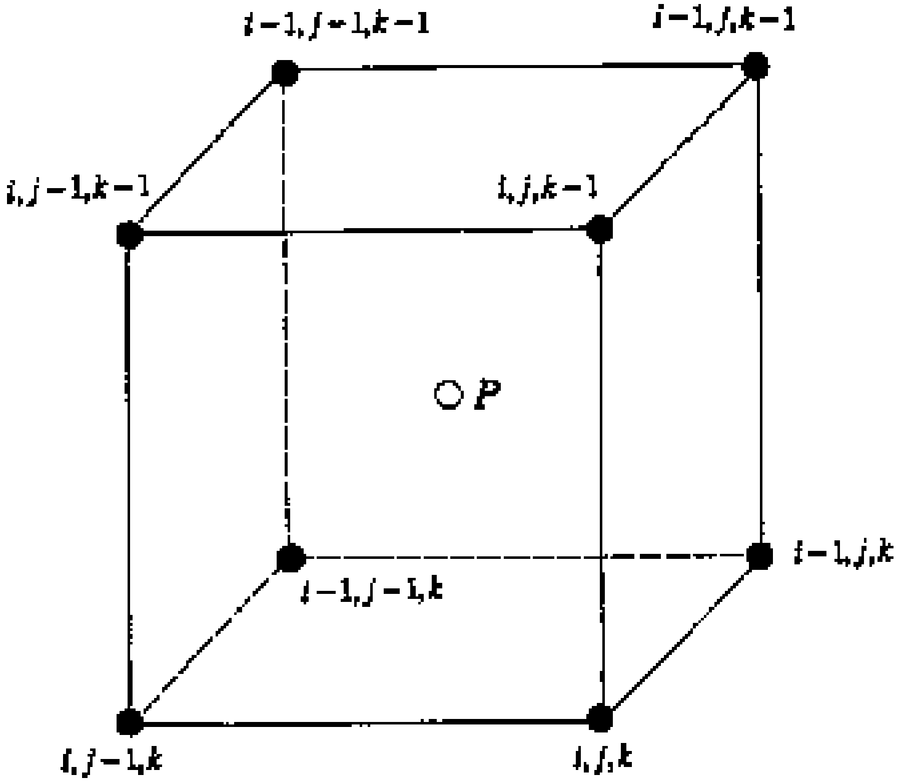
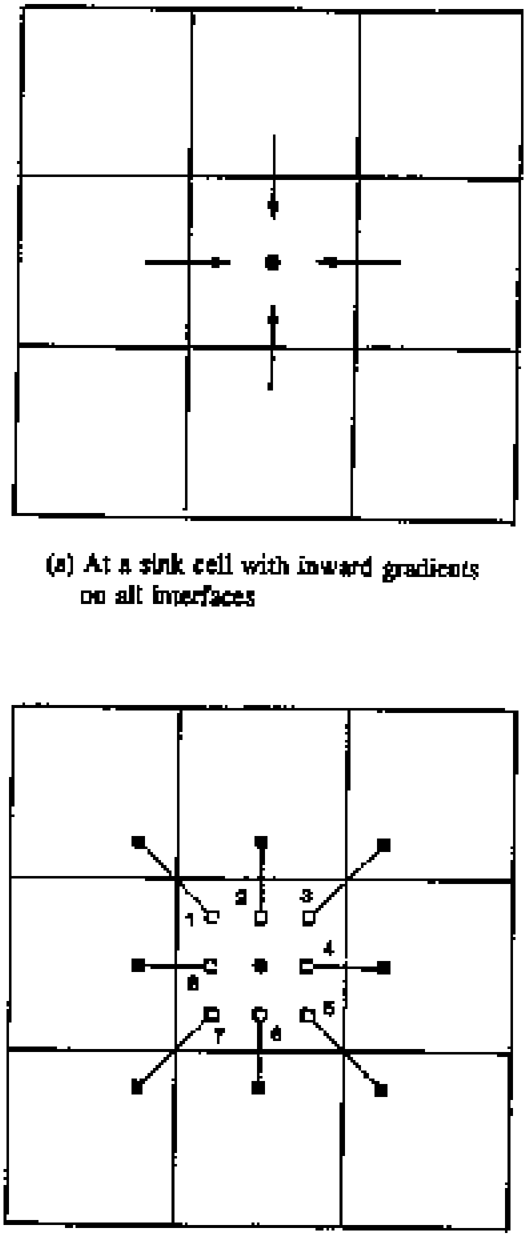


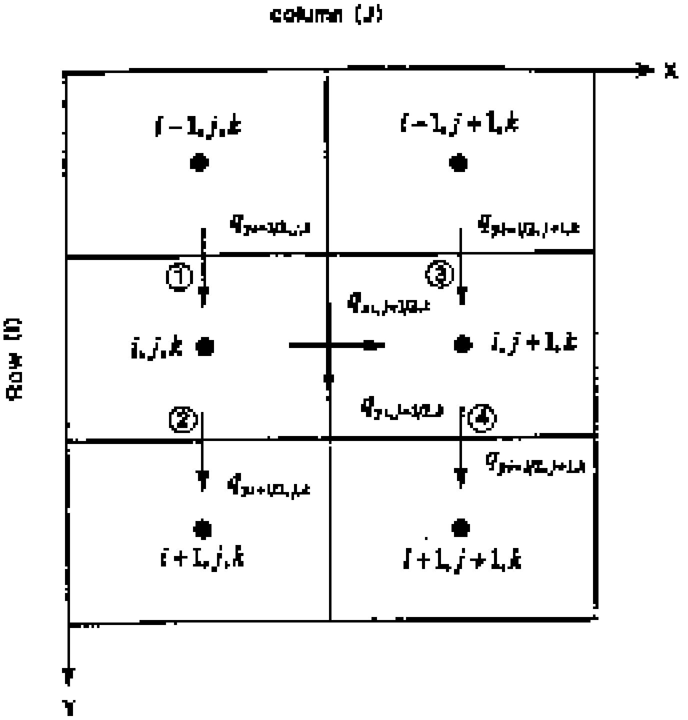
Fig. 4.11. Interpolation of the concentration at point P from the concentrations at neighboring nodes using the trilinear scheme in three dimensions.



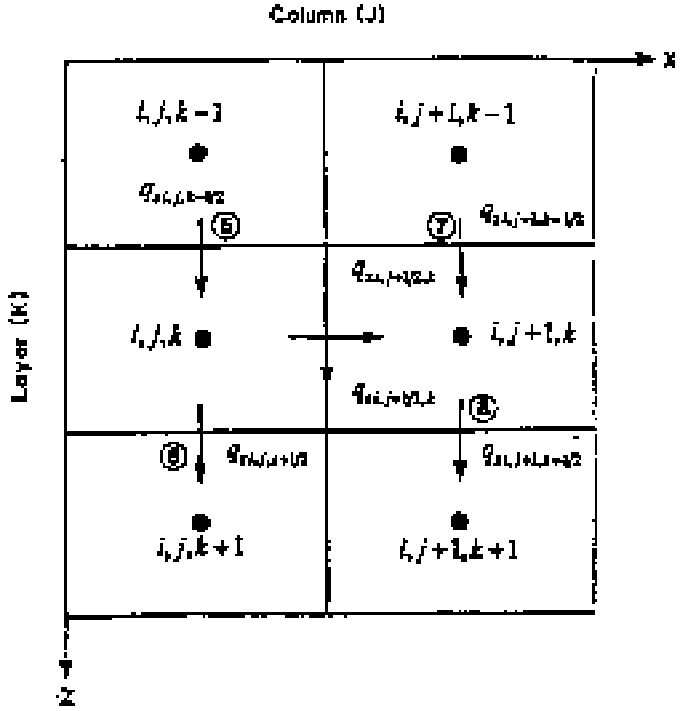
(a) At a sink cell with inward gradients on all interfaces

(b) Instead of placing one single particle at the node, multiple particles are placed and tracked backward. In this example, 8 particles distributed with a fixed pattern are used. However, both the number and the pattern can be changed in the user-specified options.

Fig. 4.12. Special treatment of sink cells in the MMOC scheme.



$q_X$ at the interface between $(i,j,k)$ and $(i,j+1,k)$ i s directly known from the flow model; $q_Y$ at the interface between $(i,j,k)$ and $(i,j+1,k)$ is interpolated from values at interfaces 1, 2, 3 and 4 in the y direction.



$q_Z$ at the interface between $(i,j,k)$ and $(i,j+1,k)$ i s interpolated from values at interfaces 5, 6, 7 and 8 in the y direction.

Fig. 4.13. Evaluation of the velocity components at the cell interfaces in the x direction for calculating components of the dispersion coefficients $D_{xx}, D_{xy}$, *and* $D_{xz}$

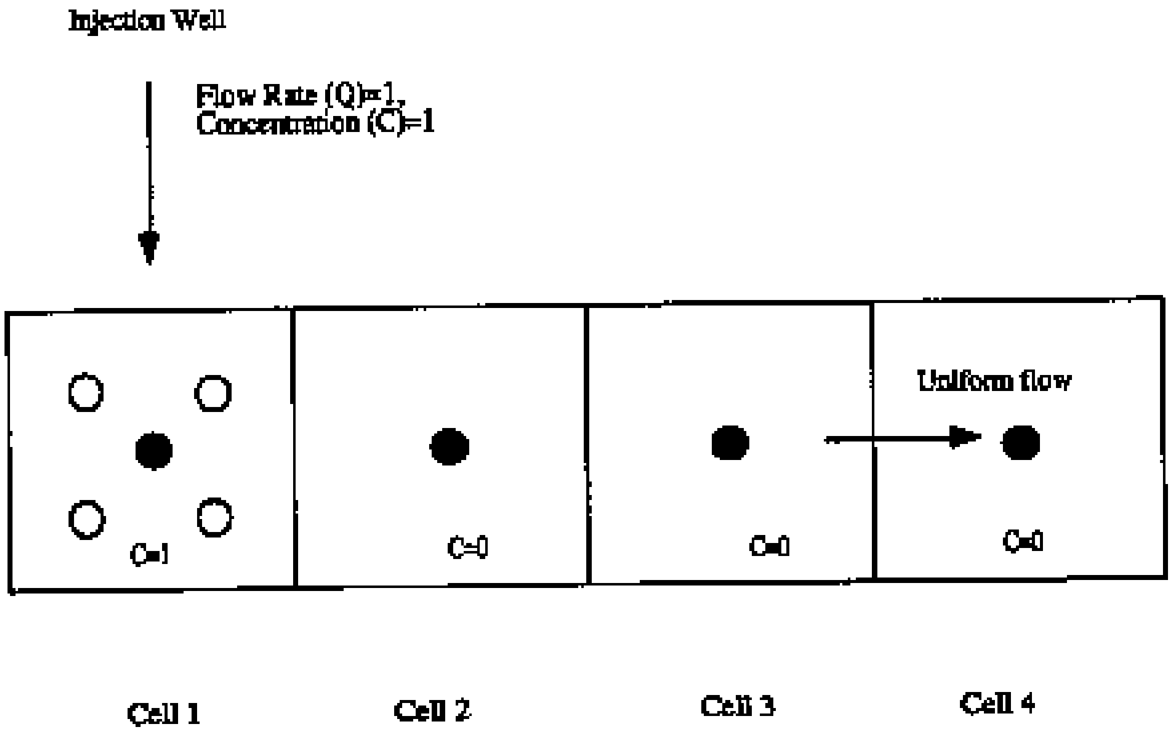


Fig. 4.14. Example of mass balance discrepancy due to discrete nature of moving particle methods.

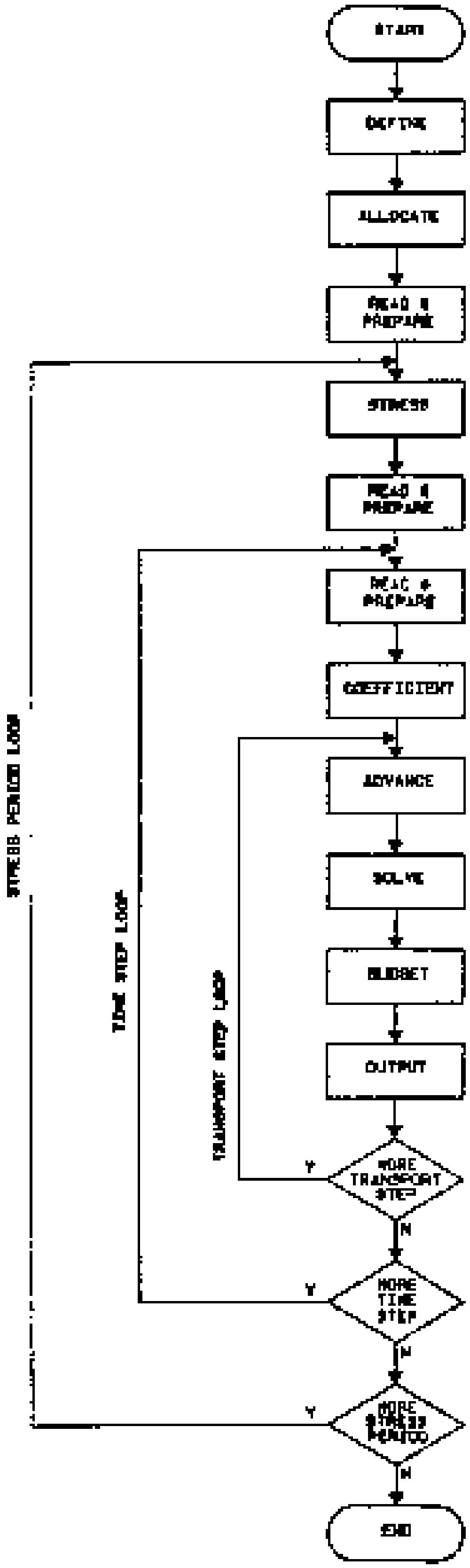
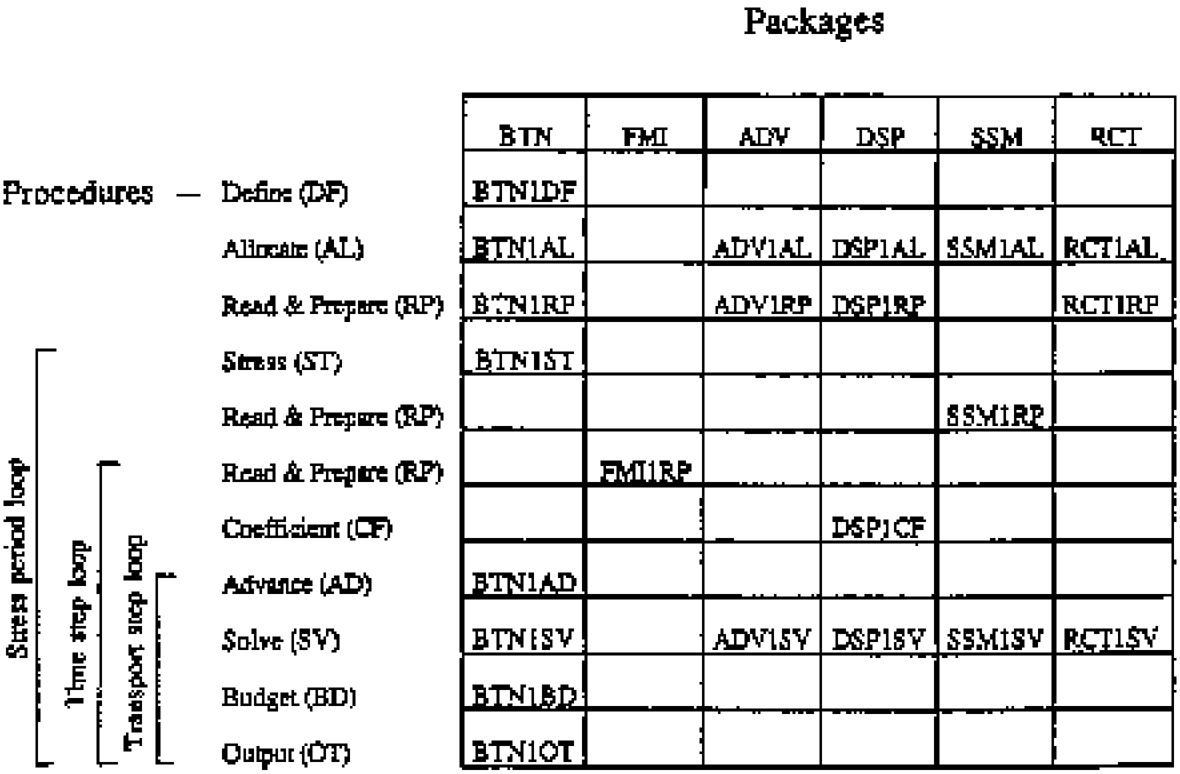
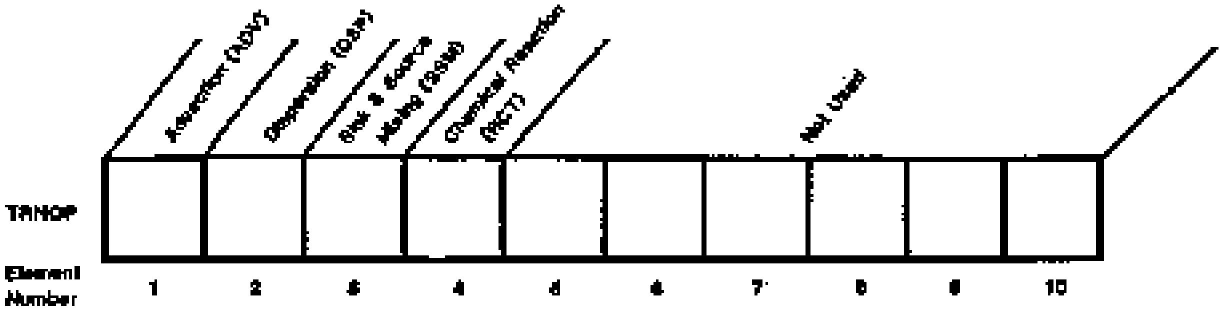


Fig. 5.1. General procedures for a typical transport simulation.



| Procedures | BTN | FMI | ADV | DSP | SSM | RCT |
|---|---|---|---|---|---|---|
| Define (DF) | BTN1DF | | | | | |
| Allocate (AL) | BTN1AL | | ADV1AL | DSP1AL | SSM1AL | RCT1AL |
| Read & Prepare (RP) | BTN1RP | | ADV1RP | DSP1RP | | RCT1RP |
| Stress (ST) | BTN1ST | | | | | |
| Read & Prepare (RP) | | | | | SSM1RP | |
| Read & Prepare (RP) | | FMI1RP | | | | |
| Coefficient (CF) | | | | DSP1CF | | |
| Advance (AD) | BTN1AD | | | | | |
| Solve (SV) | BTN1SV | | ADV1SV | DSP1SV | SSM1SV | RCT1SV |
| Budget (BD) | BTN1BD | | | | | |
| Output (OT) | BTN1OT | | | | | |

**Fig. 5.1.** Primary modules of MT3D as organized by procedures and packages.



Sample TRNOP Input Record

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| TRNOP | T | T | F | T | F | F | F | F | F | F |
| Element Number | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |

Note:
1. The Advection Option is used; an input file is needed for the Advection Package;
2. The Dispersion Option is used; an input file is needed for the Dispersion Package;
3. The Sink & Source Option is not used; no input file is needed for the Sink & Source Package;
4. The Chemical Reaction Option is used; an input file is needed for the Chemical Reaction Package;

5-10. Not used in the current version.

Fig. 5.3. Specification of the transport components to be simulated using the logical TRNOP array. The TRNOP array is entered in the input file to the Basic Transport Package.

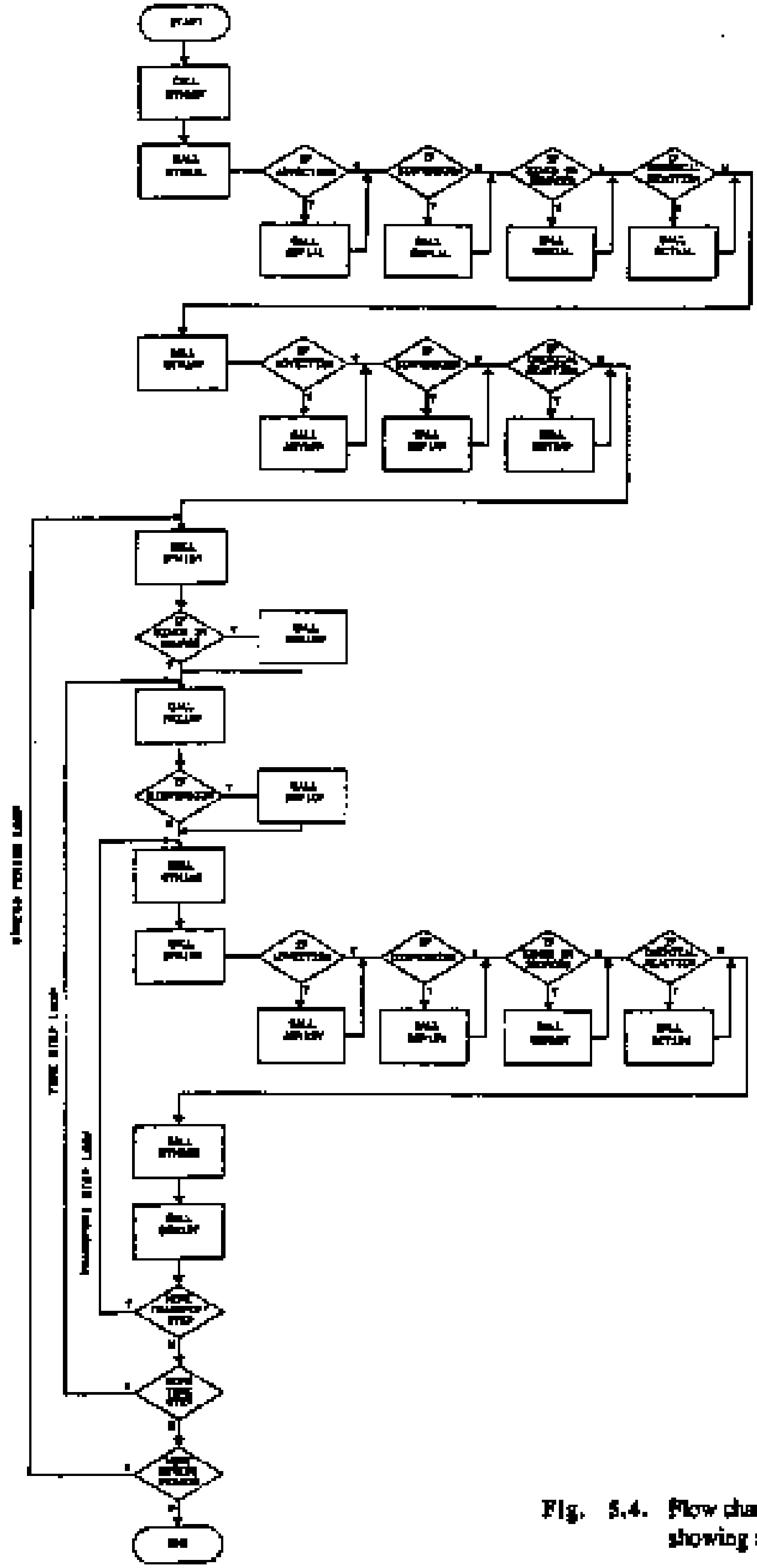


Fig. 5.4. Flow chart for the main program showing all primary modules.

```
                   CNSTNT                          FMTIN        IRPN
         IREAD
           100         0.                       (10F5.1)           3
    2.1    2.1    2.1    2.1    2.1    2.1    2.1    2.1    2.1    2.1
    2.1    2.1    2.1    2.1    2.1    2.1    2.1    2.1    2.1    2.1
   10.2   10.2   10.2   10.2   10.2   10.2   10.2   10.2   10.2   10.2
   10.2   10.2   10.2   10.2   10.2   10.2   10.2   10.2   10.2   10.2
   23.5   23.5   23.5   23.5   23.5   23.5   23.5    0.4    0.4    0.4
   23.5   23.5   23.5   23.5   23.5   23.5   23.5    0.4    0.4    0.4
   23.5   23.5   23.5   23.5   23.5   23.5   23.5    0.4    0.4    0.4
   23.5   23.5   23.5   23.5   23.5   23.5   23.5    0.4    0.4    0.4
   23.5   23.5   23.5   23.5   23.5   23.5   23.5    0.4    0.4    0.4
      0      0      0      0      0      0      0    0.4    0.4    0.4
```

(a) An array of 10 x 10 is read with the user-specified format (10F5.1) (IREAD=100).

```
           101          0.                  (FMTIN not used)           3
 5       <----------  NBLOCK
     1      10      1     10      0
     1       2      1     10    2.1
     3       4      1     10   10.2
     5       9      1      7   23.5
     5      10      8     10    0.4
```

(b) The same array as shown in (a) is read using the block format (IREAD=101).

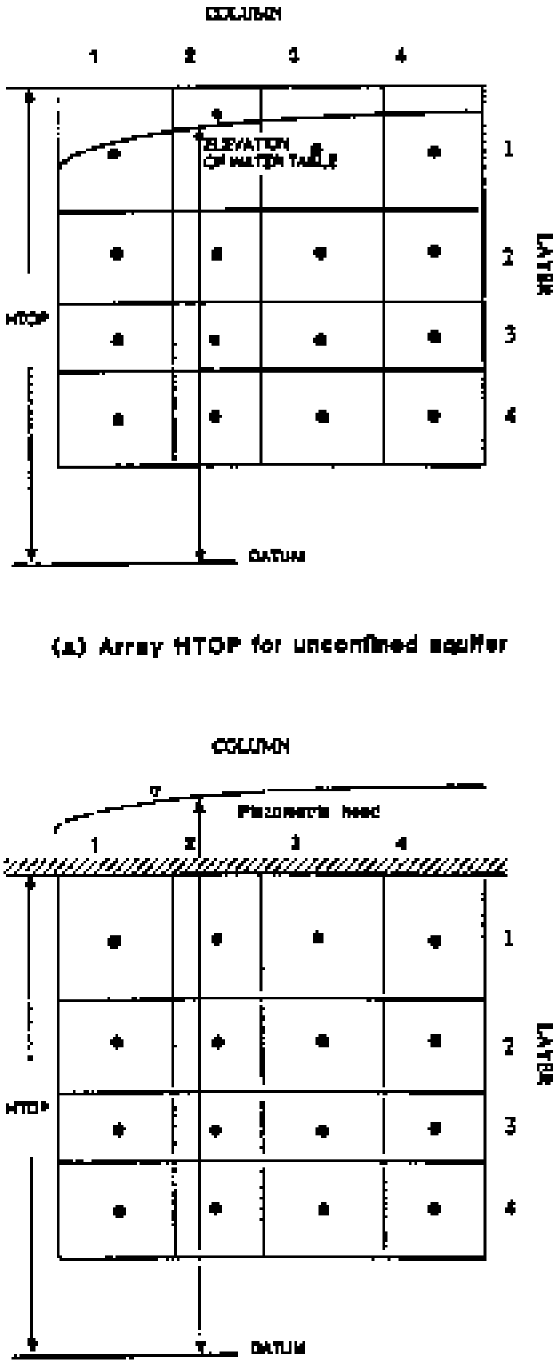
```
           102                0.                          (10F5.0)           3
 4          <---------NZONE
   2.1     10.2    23.5          0.4       <--------  ZZ(NZONE)
      1      1      1      1      1      1      1      1      1      1
      1      1      1      1      1      1      1      1      1      1
      2      2      2      2      2      2      2      2      2      2
      2      2      2      2      2      2      2      2      2      2
      3      3      3      3      3      3      3      4      4      4
      3      3      3      3      3      3      3      4      4      4
      3      3      3      3      3      3      3      4      4      4
      3      3      3      3      3      3      3      4      4      4
      3      3      3      3      3      3      3      4      4      4
      0      0      0      0      0      0      0      4      4      4
```

(c) The same array as shown in (a) is read using the zonal format (IREAD=102). Note that format (10F5.0) is used to read the zone indicators).

```
           103                0.               (FMTIN not used)              3
  20*2.1  20*10.2  7*23.5  3*0.4  7*23.5  3*0.4  7*23.5  3*0.4  7*23.5  3*0.4
  .7*23.5 . 3*0.4    7*0   3*0.4
```

(d) The same array as shown in (a) is read using the list-directed format (IREAD=103).

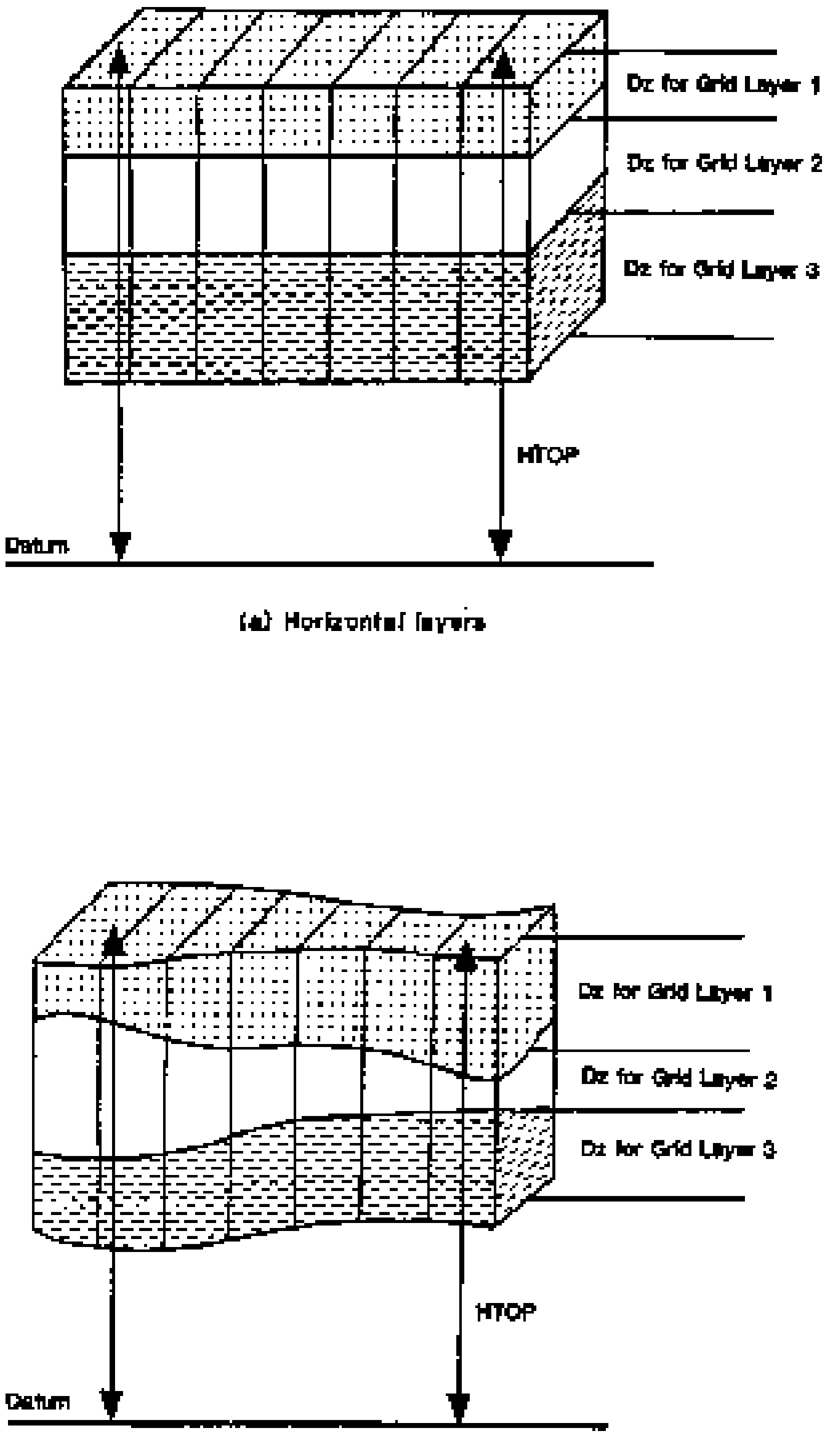
Fig. 6.1. Illustration of the various input forms used by RARRAY and IARRAY.



(a) Array HTOP for unconfined aquifer

(b) Array HTOP for confined aquifer

Fig. 6.2. Illustration of array HTOP for unconfined and confined aquifer layers.



(a) Horizontal layers

(b) Distorted layers

Fig. 4.3. Arrays HTOP and DZ for different vertical discretization schemes.

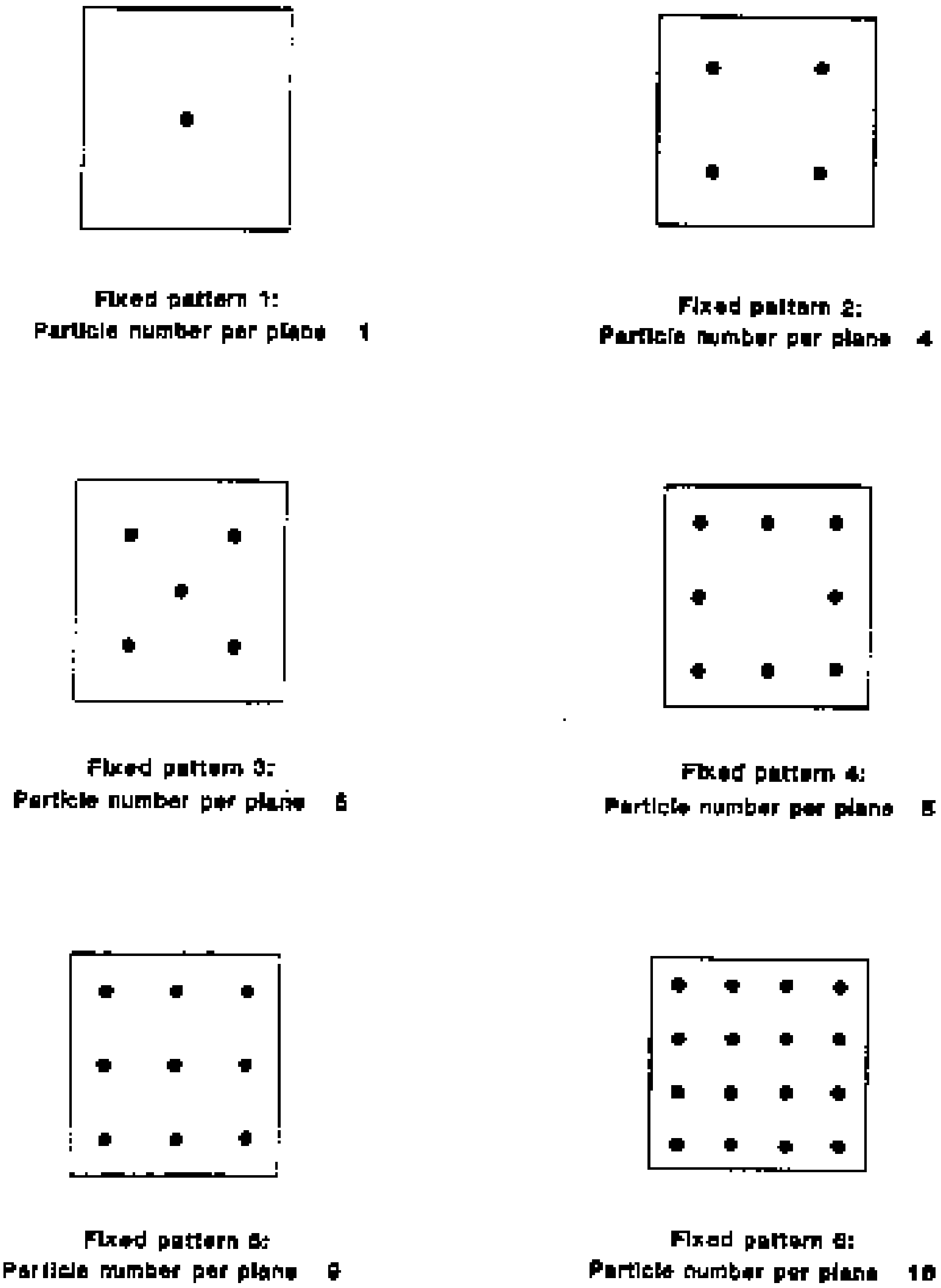
```
          1       2       3       4       5       6       7       8       9      10
         11      12      13      14      15      16      17

  1    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79
       1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

  2    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79
       1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

  3    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79
       1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

  4    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79
       1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

  5    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79
       1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

  6    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79
       1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

  7    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79
       1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79
```

(a) WRAP FORM

```
          1       2       3       4       5       6       7       8       9      10

  1    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

  2    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

  3    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

  4    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

  5    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

  6    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

  7    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

         11      12      13      14      15      16      17

  1    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

  2    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

  3    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

  4    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

  5    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

  6    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79

  7    1325.79 1325.79 1325.79 1325.79 1325.79 1325.79 1325.79
```

(b) STRIP FORM

Fig. 6.4. Illustration of wrap and strip forms of printed output for a layer containing 7 rows and 17 columns. (After McDonald and Harbaugh, 1988).



Fixed pattern 1:
Particle number per plane 1

Fixed pattern 2:
Particle number per plane 4

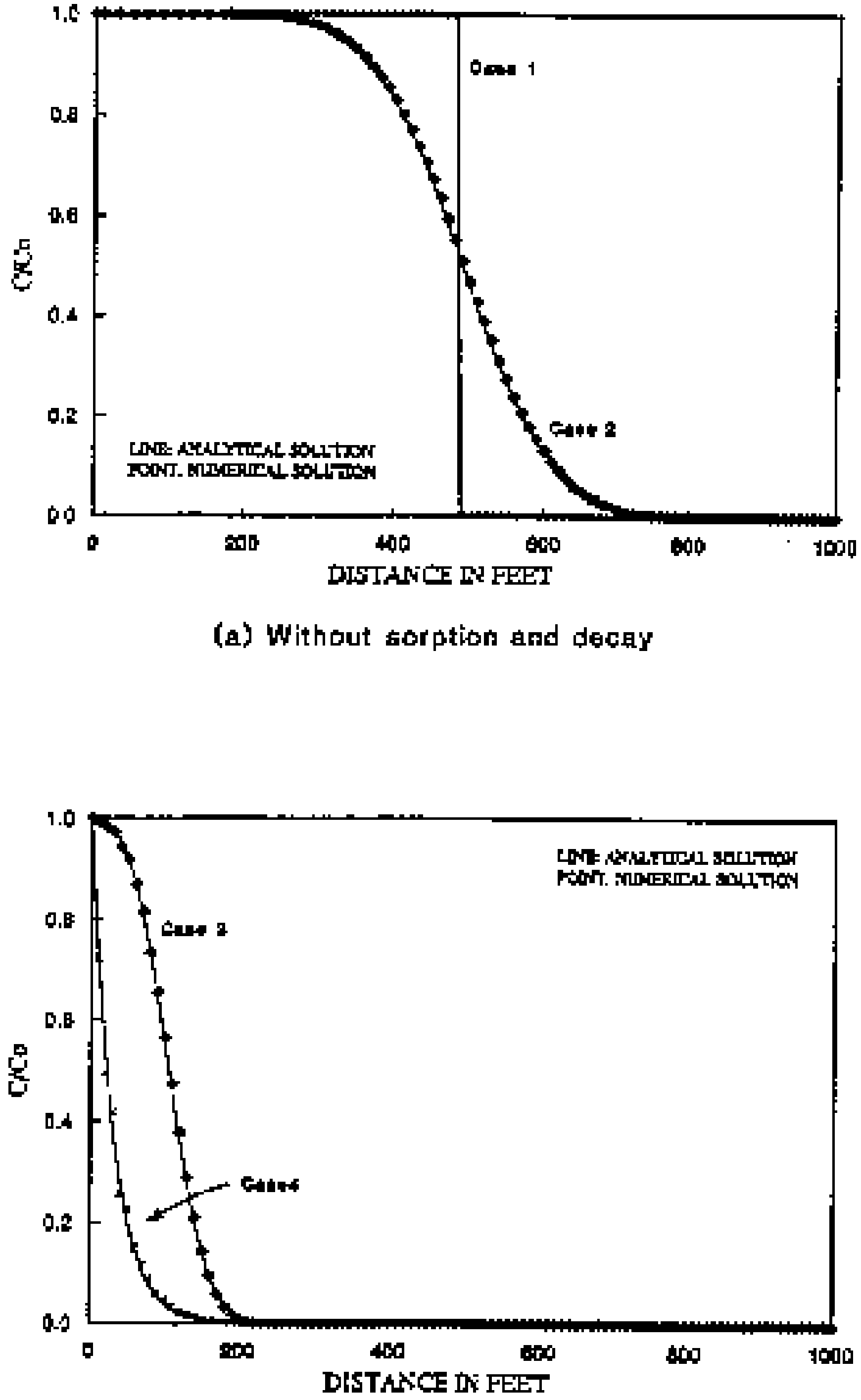
Fixed pattern 3:
Particle number per plane 5

Fixed pattern 4:
Particle number per plane 8

Fixed pattern 5:
Particle number per plane 9

Fixed pattern 6:
Particle number per plane 16

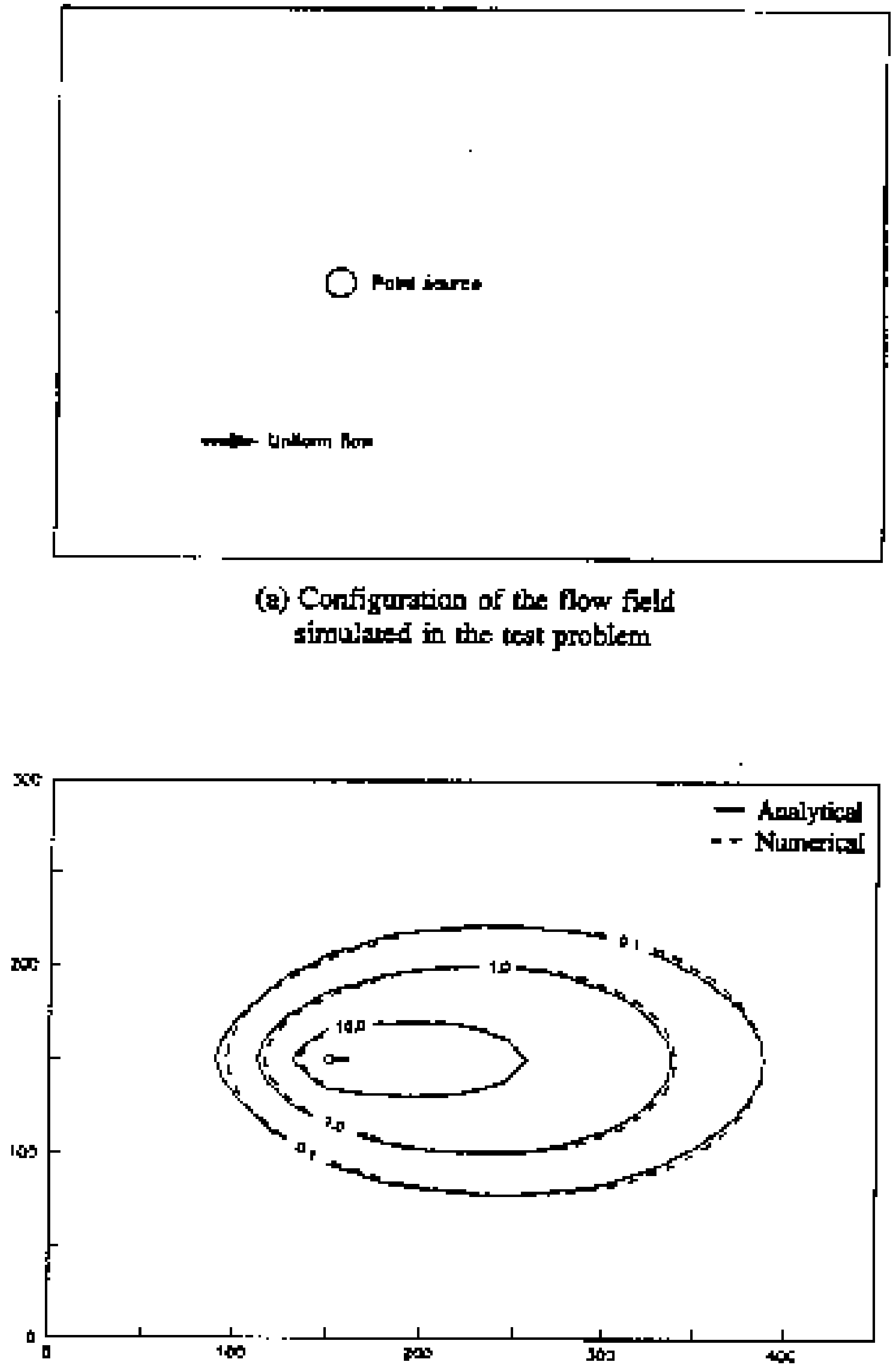
**Fig. 6.5.** Distribution of initial particles using the *fixed pattern.* If the fixed pattern is chosen, the number of particles placed per cell (NPL and NPH) is divided by the number of vertical "planes", or NPLANE, to yield the number of particles to be placed on each vertical plane, which is then rounded to one of the values shown here.



(a) Without sorption and decay

(b) With sorption and/or decay

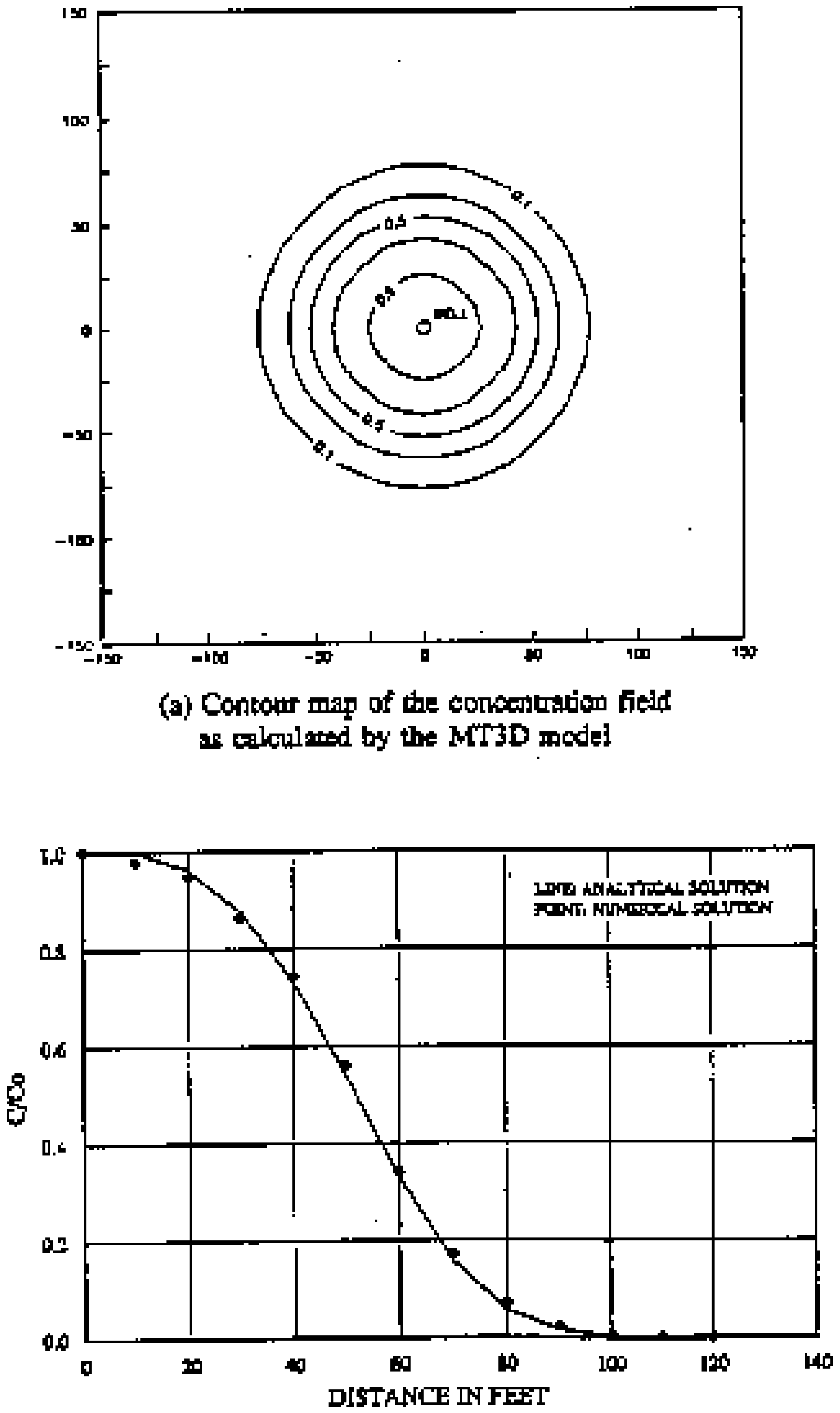
Fig. 7.1. Breakthrough curves for the one-dimensional test problem.



(a) Configuration of the flow field simulated in the test problem

(b) Concentration plume as calculated by the analytical and numerical solutions

Fig. 7.2. Comparison of the numerical and analytical solutions for two-dimensional transport from a point source in a uniform flow field.



(a) Contour map of the concentration field as calculated by the MT3D model

(b) Breakthrough curve along the X axis

Fig. 7.3. Comparison of the numerical and analytical solutions for two-dimensional transport from a point source in a radial flow field.

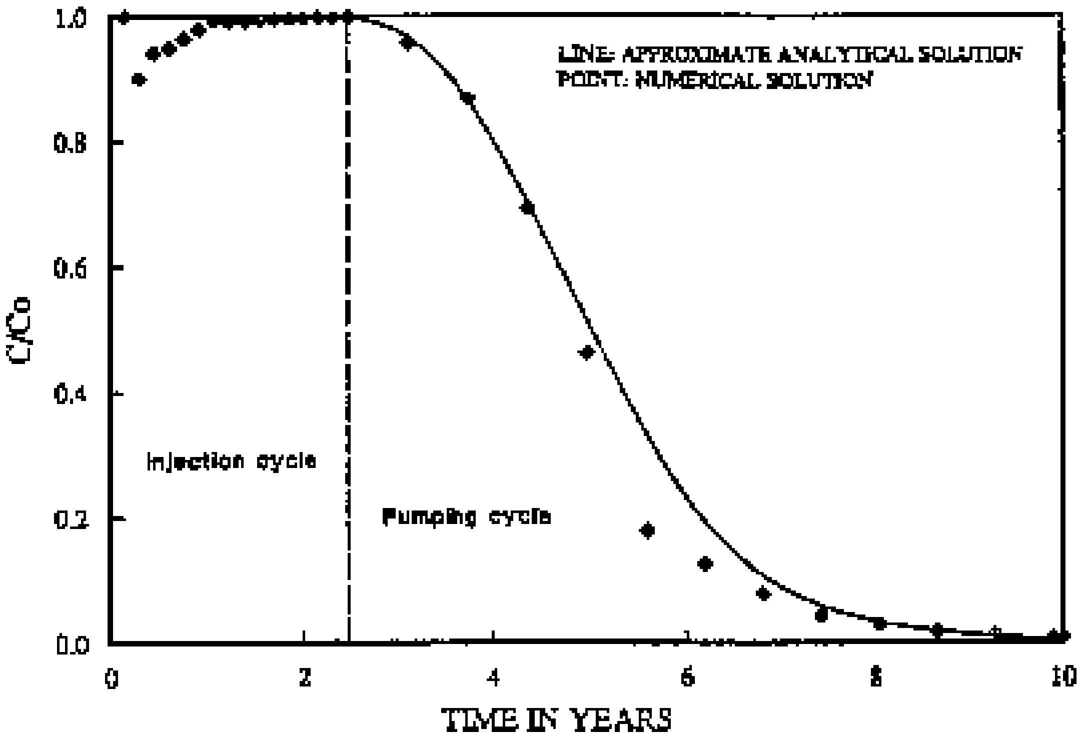


Fig. 7.4. Concentration at the well during an injection/pumping cycle as calculated by the MT3D model and the analytical solution in a strongly diverging/converging flow field.

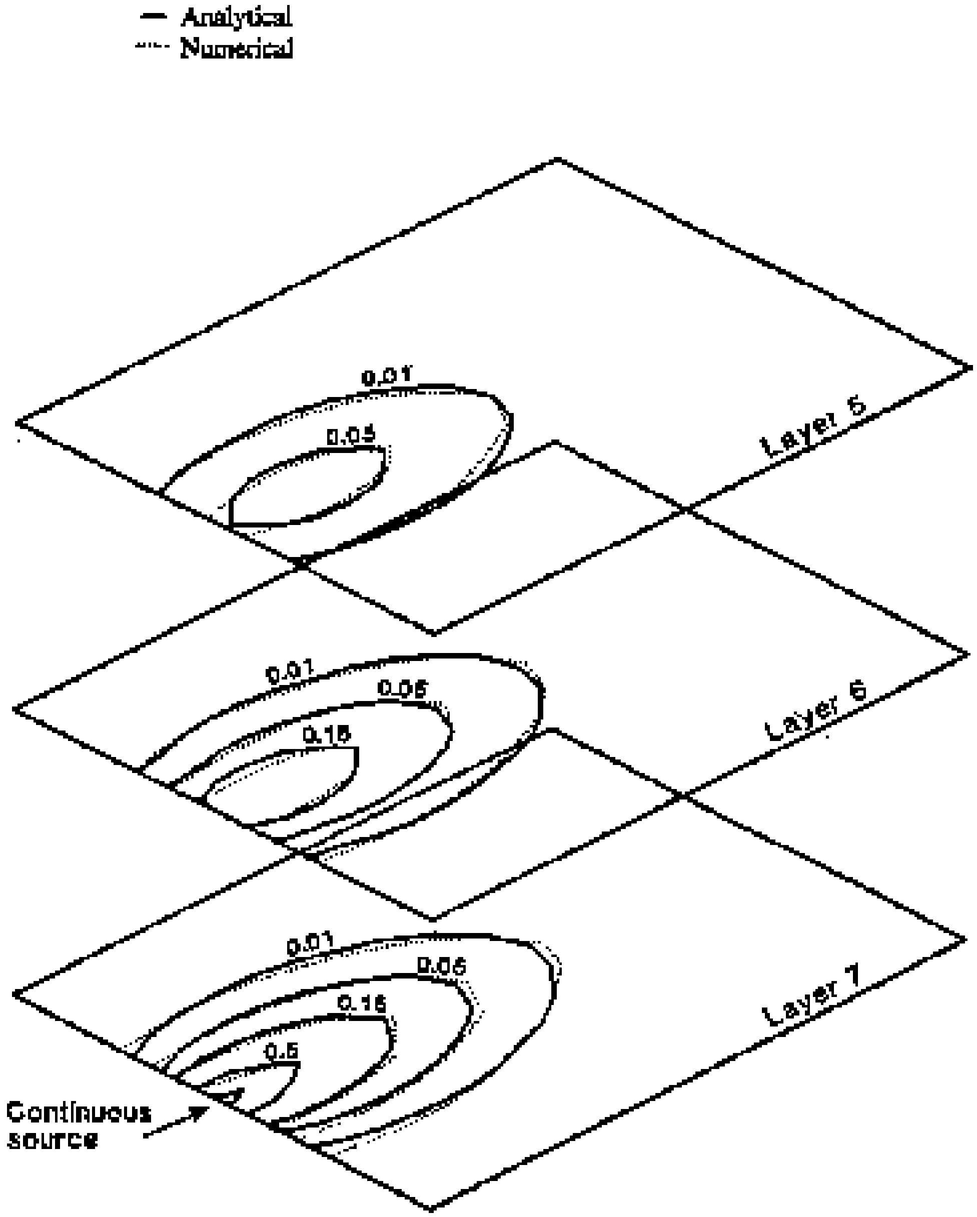


Fig. 7.5. Comparison of the numerical and analytical solutions for three-dimensional transport from a point source in a uniform flow field.

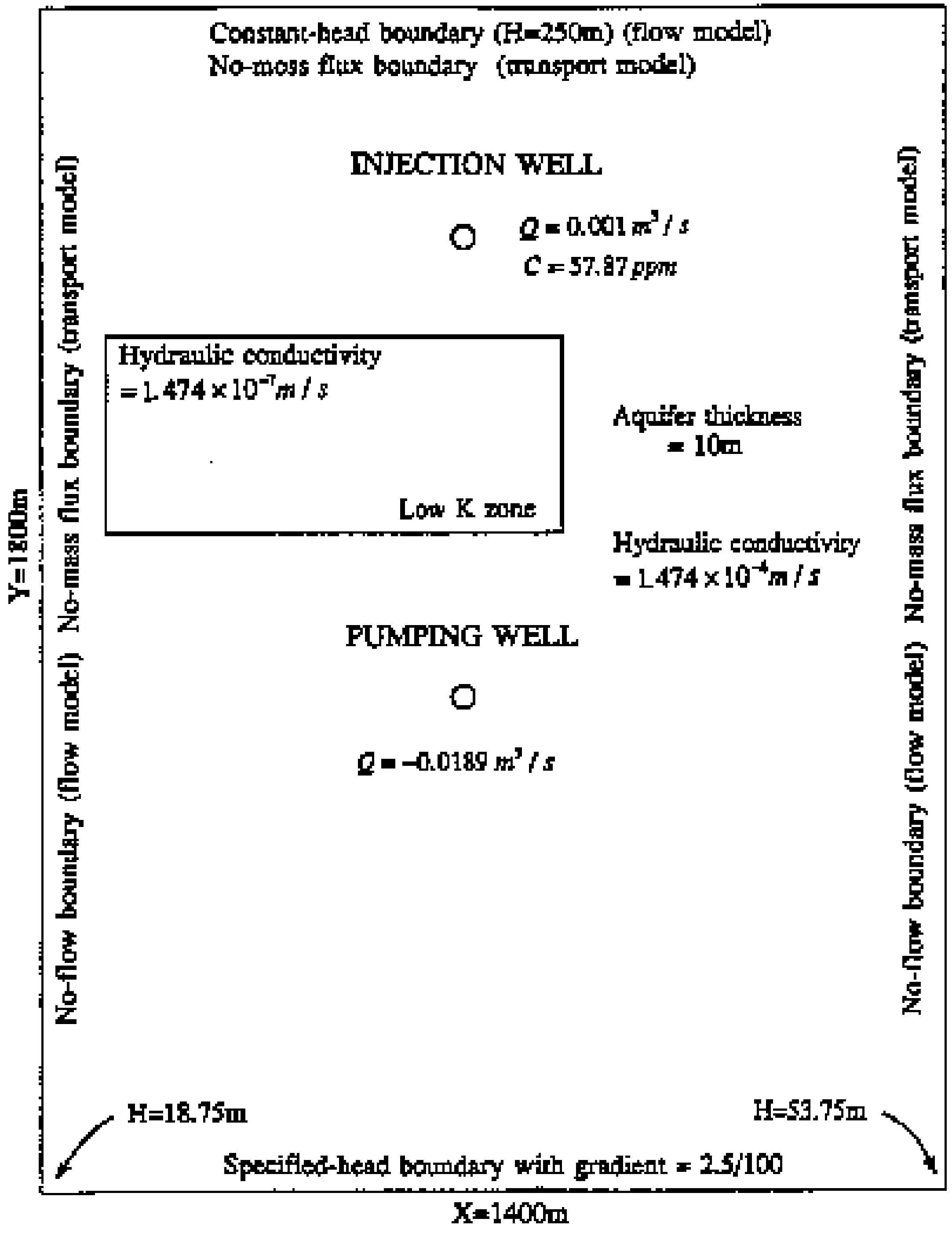

Constant-head boundary (H=250m) (flow model)
No-moss flux boundary (transport model)
INJECTION WELL
$Q = 0.001\, m^3/s$
$C = 57.87\, ppm$
Hydraulic conductivity
$= 1.474 \times 10^{-7} m/s$
Low K zone
Aquifer thickness
= 10m
Hydraulic conductivity
$= 1.474 \times 10^{-4} m/s$
PUMPING WELL
$Q = -0.0189\, m^3/s$
No-flow boundary (flow model) No-mass flux boundary (transport model)
No-flow boundary (flow model) No-mass flux boundary (transport model)
Y=1800m
H=18.75m
H=53.75m
Specified-head boundary with gradient = 2.5/100
X=1400m

Fig. 7.6. Configuration of the heterogeneous aquifer simulated in the test problem.

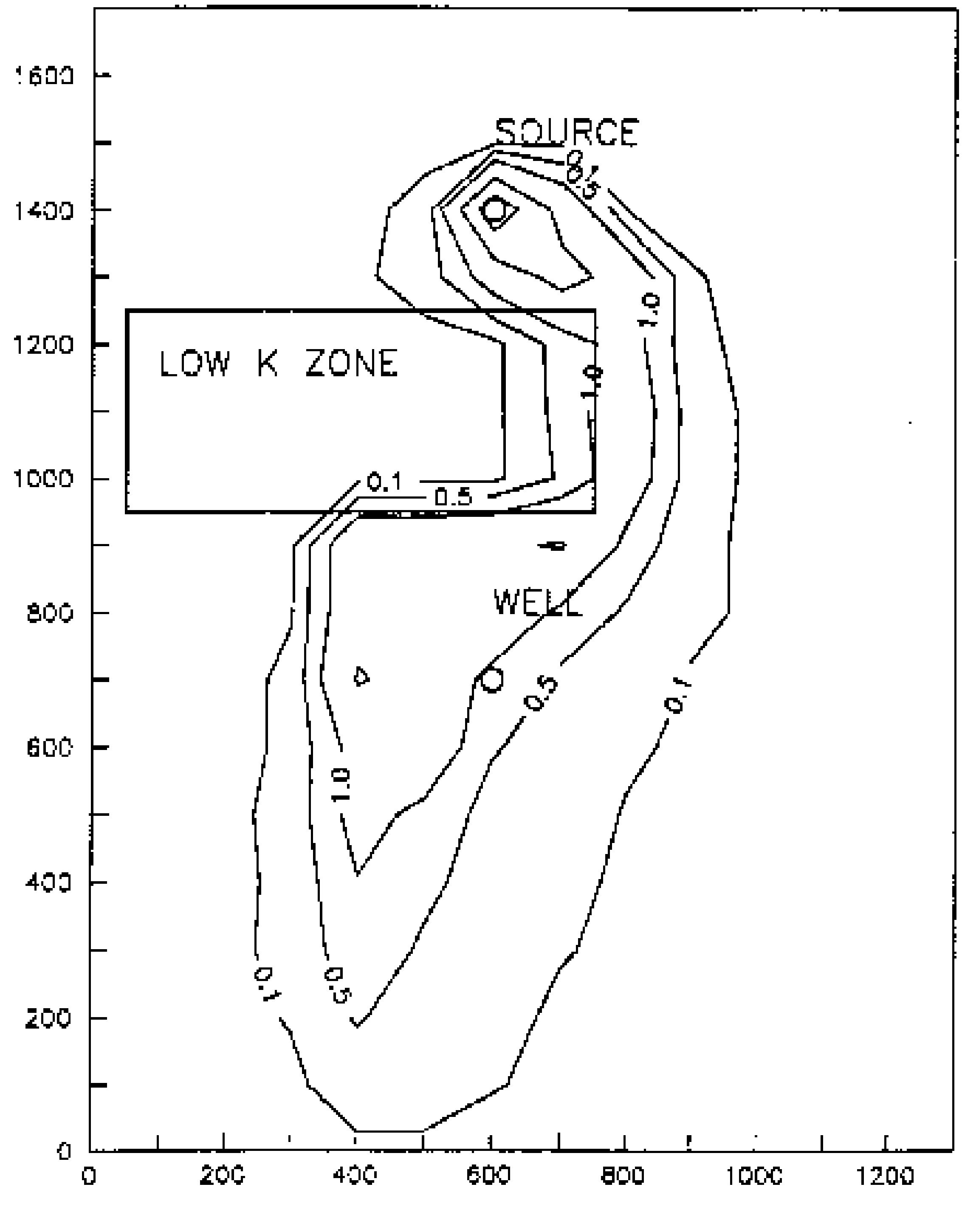


Fig. 7.7. Distribution of solute concentrations as solved by the hybrid MOC/MMOC (HMOC) solution.

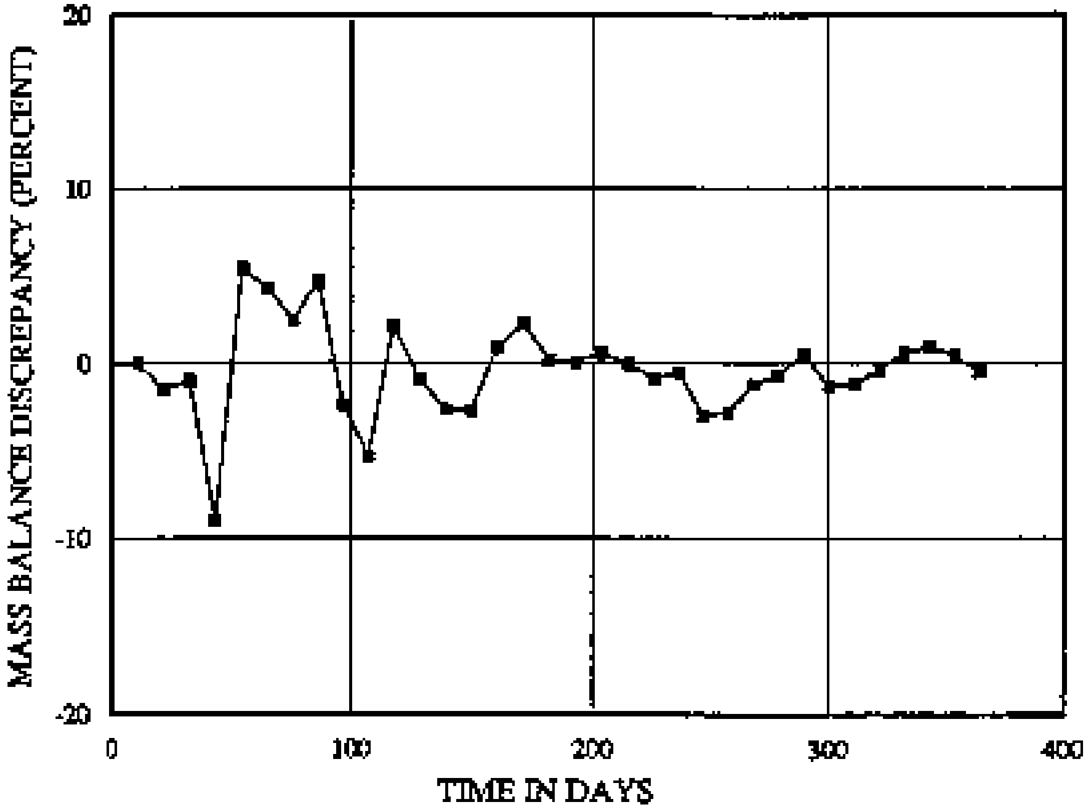


Fig. 7.8. Plot of the mass balance discrepancy error at each transport step for the test problem involving a heterogeneous aquifer.

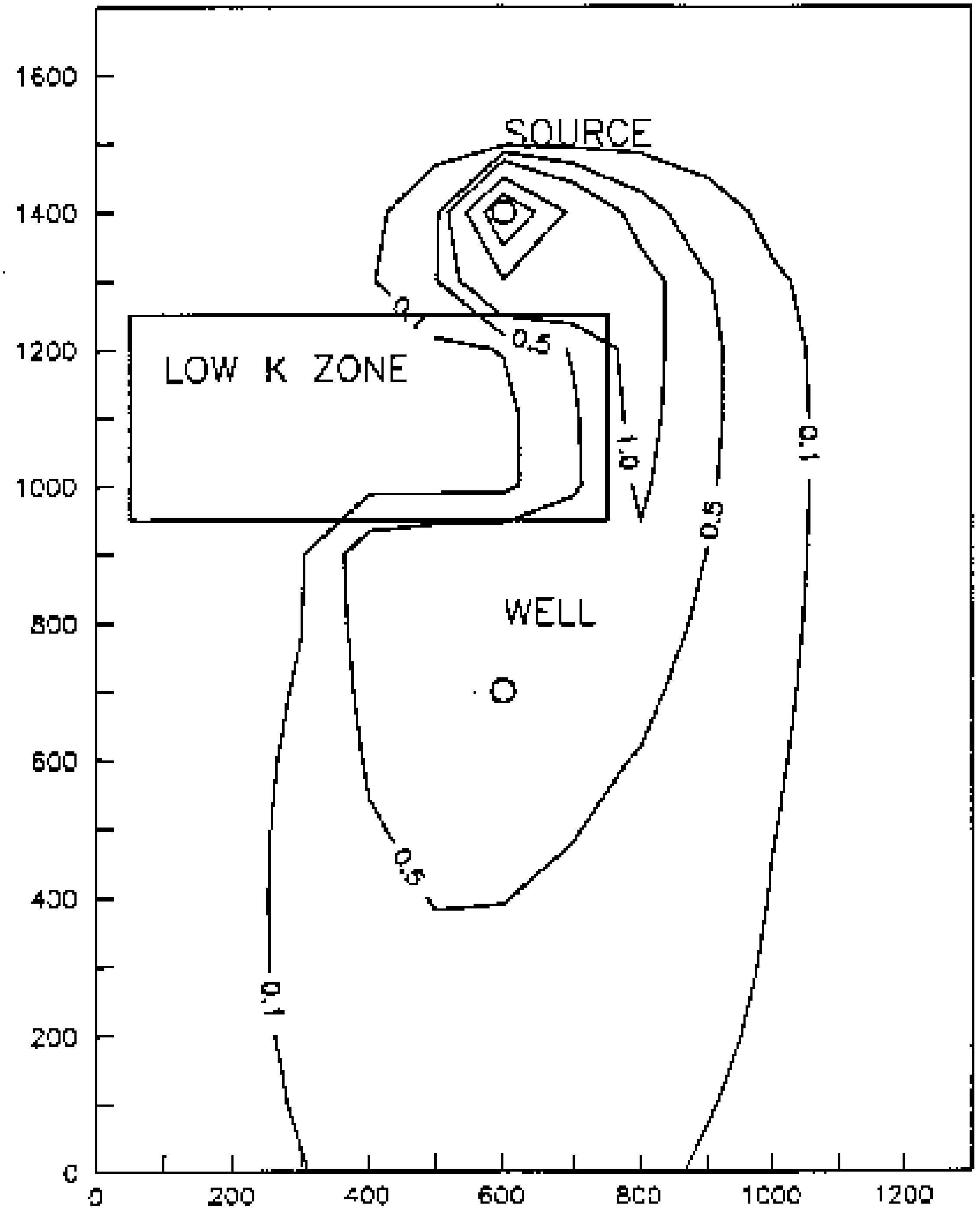


Fig. 7.9. Distribution of solute concentrations as solved by the finite difference solution for comparison with those solved by the hybrid MOC/MMOC (HMOC)solution (Fig. 7.7).

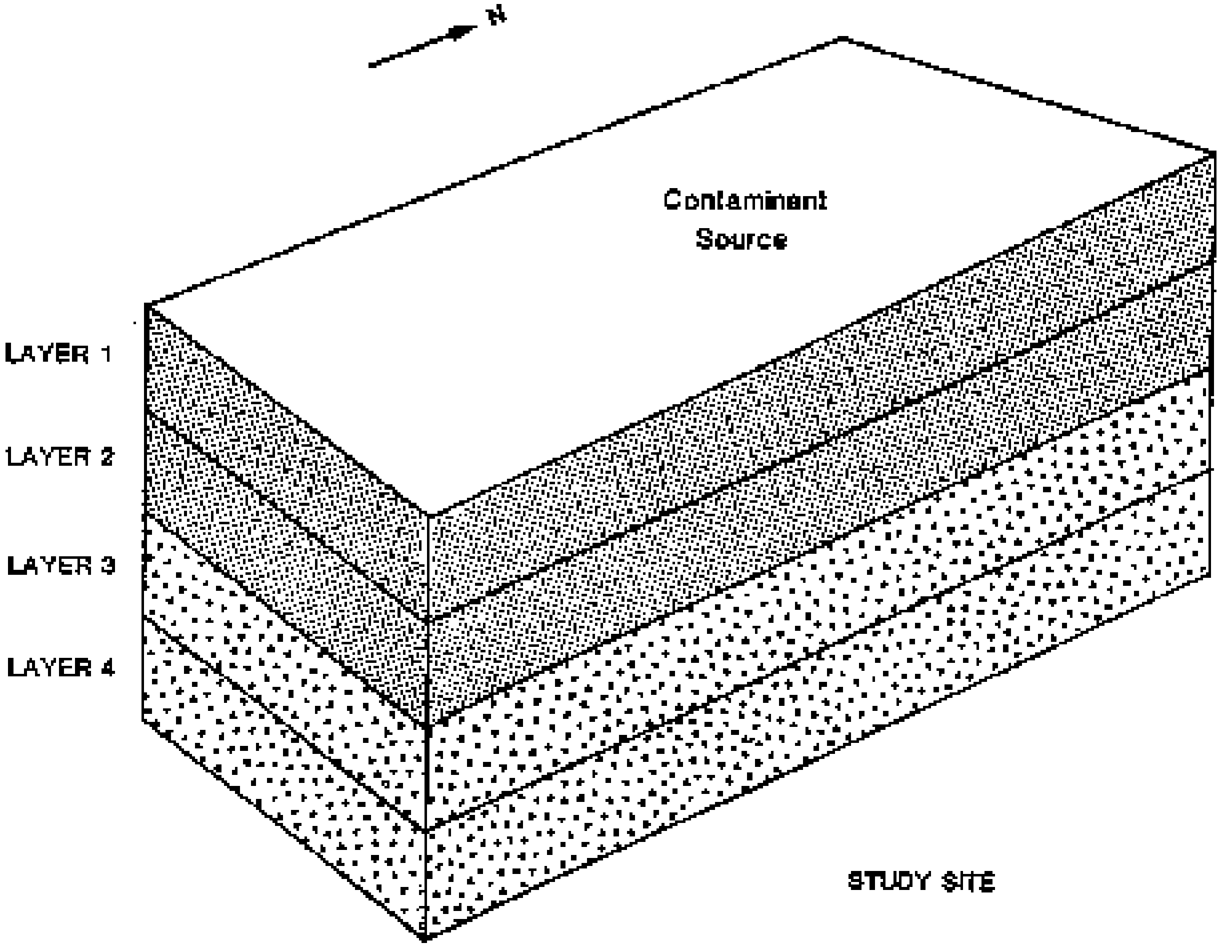


Fig. 7.10. Setting and vertical discretization in the field example.

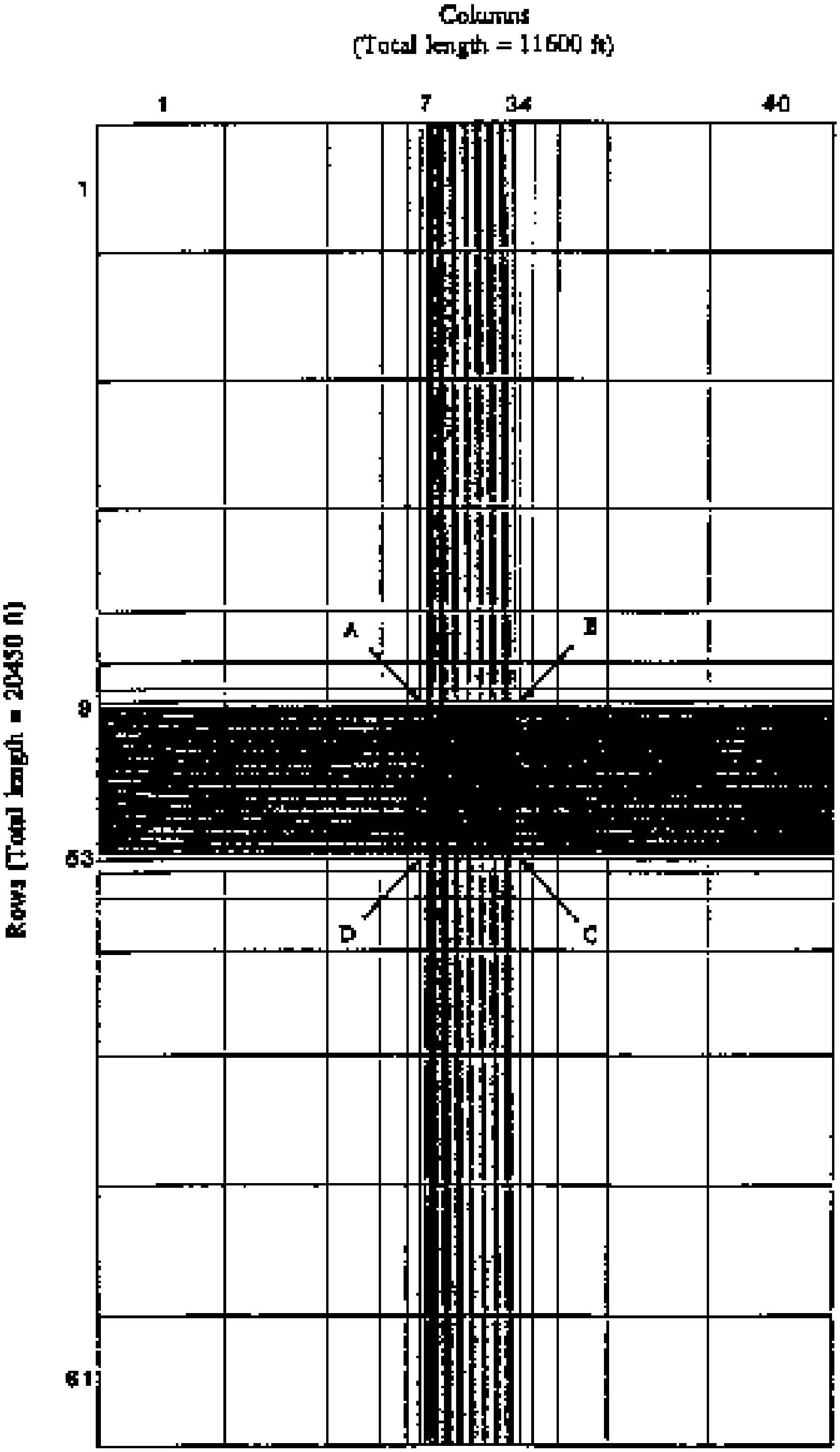
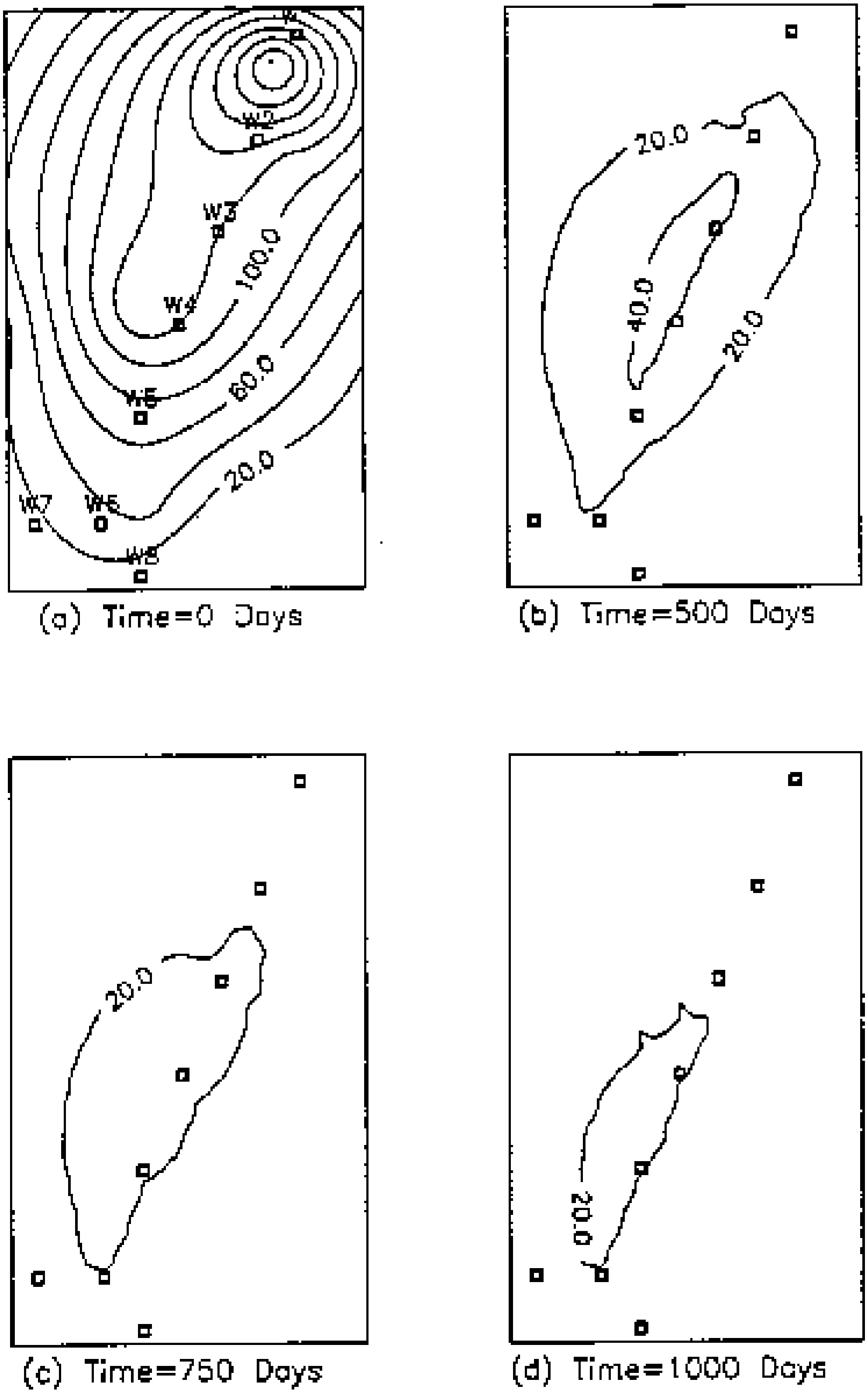


Fig. 7.11. Plan view of the finite difference mesh for the field example.



(a) Time=0 Days

(b) Time=500 Days

(c) Time=750 Days

(d) Time=1000 Days

Fig. 7.12. Present distribution of the disolved 1,2-DCA and the model-predicted concentration changes at selected times after pumping starts

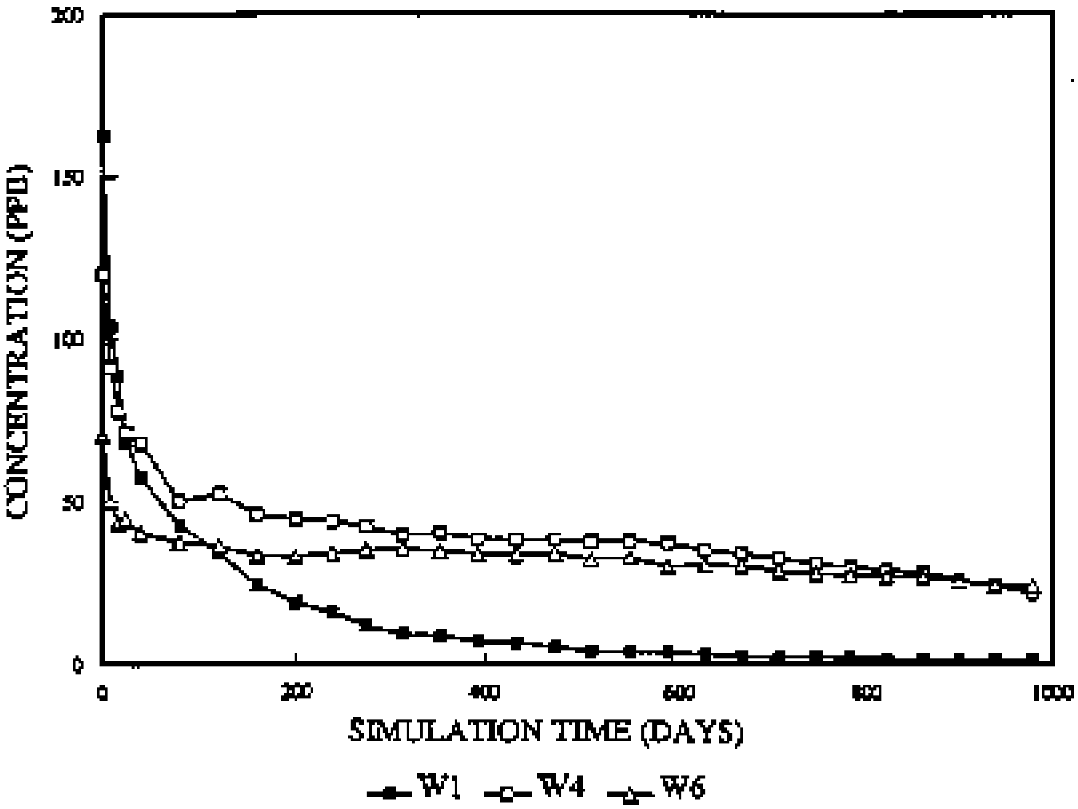


Fig. 7.13. Concentration breakthrough curves at pumping wells W1, W4 and W6, located at the northern end, middle area and southern end of the plume, respectively. (Concentrations are shown in the plot every five steps.)