NUMERICAL MODEL SIMULATIONS
AND ASSESSMENT OF CONTAMINANT
PLUME MIGRATION
REFUSE HIDEAWAY LANDFILL
MIDDLETON, WISCONSIN

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Prepared For:

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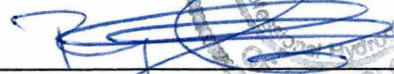101 S. Webster Street
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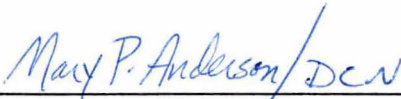Brookfield, Wisconsin 53045

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LIST OF ACRONYMS

1,2-DCE	1,2-Dichloroethylene
HSI	Hydro-Search, Inc.
MMOC	Modified Method of Characteristics
MOC	Method of Characteristics
PCE	Tetrachloroethylene
RHL	Refuse Hideaway Landfill
TCE	Trichloroethylene
VOC	Volatile Organic Compounds
WDNR	Wisconsin Department of Natural Resources
ES	Enforcement Standard
PAL	Preventive Action Limit

1.0 EXECUTIVE SUMMARY

Hydro-Search, Inc. (HSI) was contracted by the Wisconsin Department of Natural Resources in August, 1991 to perform numerical simulations of the bedrock valley sand and gravel aquifer and contaminant plume front downgradient of the Refuse Hideaway Landfill (RHL). The subject facility is located in the SW¼ of the NW¼ of Section 8, T7N, R8E, in the Town of Middleton, Wisconsin (Figure 2-1).

An earlier investigation by HSI (June, 1991) reported a contaminant plume consisting of volatile organic compounds (VOCs) has migrated approximately 3,800 feet to the southwest of the landfill within the upper 250 feet of the saturated zone (Figure 2-1). Field observations indicate that impacted ground water moves away from the landfill in the bedrock aquifer at relatively high velocity. The velocity decreases significantly farther downgradient due to decreasing hydraulic gradients and the change in medium properties from bedrock to unconsolidated sand and gravel deposits. The present extent of the contaminant plume of VOCs (Figure 2-1) encompasses two monitor wells (P-40 and P-31) within sand and gravel deposits of a bedrock valley.

Private residences exist downgradient of the plume front in the Deer Run Subdivision which is located across the bedrock valley modeled in this study. A concern addressed by this study is the potential interception of impacted ground water by these domestic water-supply wells. The model can also be used as part of a contingency plan to develop a ground-water recovery system.

Two-dimensional numerical simulations of the ground-water flow system within the bedrock valley sand and gravel aquifer were made using the U.S. Geological Survey's MODFLOW code (McDonald and Harbaugh, 1988). The contaminant transport model used to simulate plume migration was MT3D (Zheng, 1990). The flow model was independently developed and calibrated. Hydraulic heads and locations and flow rates of various sinks/sources, as solved by the flow model, were input to MT3D for subsequent plume simulations.

Flow model calibration was achieved by varying the specified head boundaries on the model's northeast and southwest boundaries (Figure 3-1). Parameters related to aquifer geometry and hydraulic conductivity (Table 3-1) are invariant. Flow model calibration resulted in an acceptable range of differences between observed/interpolated and model-calibrated hydraulic heads (Table 3-2). The water budget is balanced with a 0.00% discrepancy between inflows and outflows (Appendix C.1).

A complete calibration to match historical transport was not possible due to data limitations. Hence, it was decided to simulate 1,000 feet of the plume front and to evaluate the characteristics of the plume within the bedrock valley sand and gravel deposits on the basis of the present distribution of contaminant. Tetrachloroethylene (PCE) was simulated in the model because the chemical occurs at a higher concentration and has lower concentration standards for protection of public health than other chemicals in the plume, as defined by Chapter NR140 Wisconsin Administrative Code. A range of values for the transport parameters was simulated to analyze their effect on plume migration. Sensitivity analyses

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involved changing bedrock and sand and gravel hydraulic conductivity, longitudinal and transverse dispersivity, effective porosity, and whether or not PCE degradation occurs.

The results of sensitivity analyses used to evaluate the significance of model input parameters showed the plume's migration to be most affected by changes in hydraulic conductivity and the degree to which contaminants degrade. Parameters that had the least effect on plume movement were dispersivity and effective porosity. Increasing the concentration at the simulated source location also had negligible effects on migration rate and shape of the plume. Parameter values judged to be most representative of the study site include 30 and 10 feet for sand and gravel and bedrock longitudinal dispersivity, respectively, and 25% and 5% for sand and gravel and bedrock effective porosity, respectively. A constant PCE source of 12 parts per billion with a degradation half-life rate of 230 days was also chosen as representative of the RHL site. Because of the uncertainty in the rate of PCE degradation, model simulations were also made using a slower 730-day half-life and a "no degradation" scenario.

Simulating representative conditions (Figure 4-1 and 4-2) show that after 5 years the plume is at equilibrium with dilution, dispersion, and degradation processes, and that further migration of the PCE plume across the bedrock valley toward Deer Run Subdivision private homes is unlikely subject to uncertainties in model parameters. When simulating a slower 730-day half-life rate and higher conductivities, model results show PCE concentrations over 1 ppb at P-30 and the closest Deer Run home after 2.5 and 5 years, respectively (Figure 4-2b). Model predictions when simulating the most conservative modeled scenario (Figure 4-4) of higher conductivities and no degradation (considered unrepresentative of the site) show PCE concentrations over 1 ppb arriving at well P-30 after 2 years, at the nearest private home after 4 years, and at well P-41 after 9 years (Table 4-1). Simulations of representative conditions and assuming the source is removed show all PCE concentrations within the valley are non-detectable after approximately 2 years.

Evaluation of the routine monitoring strategy using the most conservative modeled scenario suggests the placement of a new sentry well near the middle of the bedrock valley (Figure 4-39). Based on PCE arrival times, monitor well sampling could be scheduled on a semi-annual or annual frequency.

In conclusion, any remedial or monitoring decisions based on this modeling effort should account for the reality that model results reflect the constraints and assumptions that are present concerning the numerical representation of the real hydrogeologic system and its hydraulic boundaries at the site. Model results suggest that migration of PCE across the valley is unlikely but cannot be considered conclusive due to the inherent uncertainties in transport parameters simulated in this analysis.

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2.0 INTRODUCTION

2.1 Overview

Hydro-Search, Inc. (HSI) was contracted by the Wisconsin Department of Natural Resources in August, 1991 to perform numerical simulations of the bedrock valley sand and gravel aquifer and contaminant plume front downgradient of the Refuse Hideaway Landfill (RHL). The subject facility is located in the SW¼ of the NW¼ of Section 8, T7N, R8E, in the Town of Middleton, Wisconsin (Figure 2-1).

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Private residences exist downgradient of the plume front in the Deer Run Subdivision which is located across the bedrock valley modeled in this study. A concern addressed by this study is the potential interception of impacted ground water by these domestic water-supply wells.

2.2 Objectives

The objectives of the ground-water model include the following:

♦   Simulate the in-field hydrogeologic and contaminant concentration conditions;

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♦ Evaluate the distance at which dispersion, dilution, and degradation would relegate the plume moving through the bedrock valley to non-detectable levels, and the time required for this to occur with and without a source of contaminant;

♦ Evaluate the concentrations and conditions required for contaminants to reach residential areas and whether or not those conditions are likely to exist; and

♦ Evaluate the current routine monitoring strategy and selected monitor well sampling locations near the landfill for long-term monitoring.

The model can also be used as part of a contingency plan to develop a ground-water recovery system. Information that could be obtained through model simulations include optimal placement of well locations and pumping rates required to create a sufficient radius of influence to remove impacted ground water and prevent further migration.

The scope of the modeling effort was based upon recommendations made by HSI to the WDNR in a proposal dated May, 1991 and included six tasks. These tasks included development of the conceptual model and data input files, the representation of model input and output, model calibration and simulation, sensitivity analyses, and the interpretation and reporting of results. This report presents documentation of project modeling methodology and conclusions, as well as HSI's assessment of plume migration.

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3.0 SCOPE OF MODELING WORK

3.1 Description of Numerical Models

3.1.1 Ground-Water Flow Model

Numerical simulations of the bedrock valley sand and gravel aquifer were made using the U.S. Geological Survey's MODFLOW code (McDonald and Harbaugh, 1988) which is a widely used numerical model for evaluating ground-water flow problems. MODFLOW simulates steady and transient flow for either two or three-dimensional irregularly-shaped aquifer systems. Ground-water flow within the aquifer is simulated using a block-centered finite-difference approach. Layers can be confined, unconfined, or a combination of both. Flow from external stresses, such as flow to wells, areal recharge, evapotranspiration, flow to drains, and flow through river beds, can also be simulated.

Hydraulic conductivities or transmissivities for any layer can differ spatially and be anisotropic; grid axes should be aligned with the principal directions of the hydraulic conductivity tensor. Specified head and specified flux boundaries can be simulated, as well as head dependent flux boundaries which supply a source of water to the model from outside a model boundary. Documentation for MODFLOW is presented in Appendix A.1.

The MODFLOW program used for this project utilizes the strongly implicit procedure which provides a fast method for solving the associated matrix of governing equations. In addition, HSI has also made minor changes to the computer code to facilitate interpretation of model results and to develop contour maps of measured data and model-simulated output. These changes involve the generation of model output in a data format that can be accepted by Surfer (Golden Software, 1990).

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3.1.2 Transport Model

The contaminant transport model used to simulate plume migration was MT3D (Zheng, 1990) which is a comprehensive three-dimensional solute transport model for simulation of advection, dispersion, sink/source mixing, and chemical reactions of contaminants in ground-water systems. The MT3D transport model can be used in conjunction with any block-centered finite-difference flow model, such as MODFLOW, and is based on the assumption that changes in ground-water chemical concentration will have negligible effects on the flow field. Therefore, the flow model for this study was independently developed and calibrated. A Flow Model Interface Package is used to link the flow model (MODFLOW) and MT3D whereby an unformatted file consisting of heads, fluxes across cell interfaces in all directions, and locations and flow rates of various sink/sources, as solved by the flow model, are retrieved and used by MT3D for transport simulations. MT3D documentation is presented in Appendix A.2.

According to Zheng (1990), the numerical solution implemented in MT3D is a mixed Eulerian-Lagrangian method. The Lagrangian part of the method is used for solving the advection term and has three basic solution options: (1) the method of characteristics (MOC), (2) a modified method of characteristics (MMOC), and (3) a hybrid of these two methods which combines the strength of MOC for eliminating numerical dispersion (at sharp concentration plume fronts where advection dominates) with the computational efficiency of MMOC (at smooth concentration fronts where less advection and dispersion and chemical reactions take place). The Eulerian part of the method is used for solving the dispersion and chemical reaction terms, and utilizes a conventional block-centered finite-difference approach. The accuracy of the MT3D model has been verified for simple problems where analytical solutions are available, and for more complicated field problems involving evaluation of the effectiveness of proposed ground-water remediation schemes (Zheng, 1990).

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3.2 Conceptual Model Development

The hydrogeology of the RHL site and extent of contaminant migration is described in an earlier report by HSI (June, 1991). Based on the results of HSI's field investigation, a conceptual model was developed to present a qualitative representation of the natural system at the RHL. In consultation with the WDNR, the model effort was focused on the sand and gravel deposits within the bedrock valley (Figure 2-1) where the leading edge of the downgradient contaminant plume occurs. A two dimensional representation of the system was selected. A complex three-dimensional (more than one layer) representation of the study area was not considered technically or economically justified due to the limited field data. A one-layer numerical model was, therefore, chosen as a viable balance between model complexity and availability of field data. However, a contrast in hydraulic conductivity was modeled to account for flow of ground water within both the bedrock and the valley deposits.

The present PCE plume front is simulated as u-shaped and comprises 131 point source nodes located in cells within the plume extent contour in Figure 3-1. These cells were simulated both as constant and variable sources during sequential prediction runs. The actual plume could be asymmetrical and extend farther toward well P-41 due to steeper gradients (Figure 3-2) and the direction of regional ground-water flow. However, the shape of the simulated plume is based on the known extent of tetrachloroethylene (PCE) concentrations in ground water as observed in wells P-40 and P-31. The actual monitor well locations within the model grid are entered in MT3D as observation points where concentrations at each transport step are calculated and printed in the output. The input files for the transport model are found in Appendix B.2.

As with any model development, certain assumptions were made regarding the representation of the hydrogeologic and ground-water flow system. These assumptions concern the in-field hydrogeology and contaminant movement and include the following:

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♦ Recorded/measured data from monitor wells P-30, P-31, P-39, P-40, and P-41 are representative of sand and sand and gravel aquifer conditions over the entire modeled area. Although the locations from which to calibrate the model are few, the above monitor wells are located within the modeled area of interest and are reasonably distributed across the model grid (Figure 3-1);

♦ Hydraulic properties of the bedrock within the modeled area are similar to those reported in previously published literature;

♦ Sand and gravel deposits are confined or semi-confined, relatively homogeneous, and isotropic;

♦ No significant upward or downward vertical gradients exist between the sandstone/dolomite bedrock that underlies the unconsolidated sediments and the sand and gravel deposits themselves;

♦ Observed head distribution in January, 1991 is representative of the long-term and/or average areal gradient. The potentiometric surface is most likely near its lowest levels during this period. Little site-specific information exists on how seasonal variations affect aquifer conditions. However, any changes are most likely uniform across the model area, and would not significantly affect aquifer flow/transport characteristics;

♦ No other source of water contributes to ground-water flow within the confined sand and gravel aquifer in the modeled area besides regional flow within bedrock and sand and gravel.

These assumptions conform reasonably well to the observed conditions in the field. The principal reasons for not simulating ground-water recharge to the sand and gravel aquifer by way of precipitation or Black Earth Creek are stated below:

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- The sand and gravel aquifer is confined or semi-confined by a surficial clay/silt layer that is present across the bedrock valley in the area of interest;

- Field data indicate that Black Earth Creek is hydraulically connected to mainly shallow ground water, that the connection is variable, and that the majority of the stream is gaining;

- No surface water samples contained detectable VOCs; and,

- No VOCs were detected in water-table well P-31S, screened within the clay/silt layer adjacent to Black Earth Creek indicating separation of shallow ground-water flow from impacts in the deeper portions of the sand and gravel.

3.3 Model Development and Data Input Files

A numerical model was chosen over an analytical solution because an accurate prediction of the spatial variability in the ground-water velocity field is critical to an accurate transport solution. At this site, advection is the dominant process controlling the direction of contaminant transport. Analytical models accept only one value for ground-water velocity. Such a simplification would over-simplify the hydraulics of the RHL site. A single ground-water velocity value assumes a constant hydraulic conductivity and gradient, and effective porosity.

The plume front and surrounding region was discretized into 20 rows, 50 columns, and one layer. The grid is comprised of 1,000 nodes covering a total area of 16,822,000 square feet (1,563,615 square meters; Figure 3-1). All model cells are 100 feet in the northeast-southwest direction. Cell size in the northwest-southeast direction for the last seven columns on each of the model's shorter boundaries have dimensions increasing outward of 150, 225, 337, 505, 757, 1,135, and 1,702 feet. The paucity of site-specific data did not justify the use of smaller-sized cells. The origin of the Cartesian coordinate system of cells is located at the upper left or most northern corner cell which starts the first row, first column, and layer,

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or cell (1,1,1). This same spatial discretization convention is used by MODFLOW and MT3D.

Model grid axes are generally aligned with the principal flow direction. No flow boundary conditions are assigned for the shorter northwest and southeast model boundaries which are located at a distance (approximately 1 mile) from the source location so that the transport solution within the modeled plume area is not affected by boundary conditions. Specified heads were assigned to the longer northeast and southwest model boundaries throughout the steady-state calibration and prediction runs. Specified flux boundaries were to be assigned to these longer model boundaries in the event any transient simulations were made to predict ground-water recovery system performance.

To simulate the historical transport of the RHL plume accurately, the entire area encompassed by the plume would have to be modeled. Furthermore, an accurate calibration of the plume's characteristics requires knowledge of the locations, timing, and strengths of contaminant sources from the time of initial ground-water contamination by the landfill. Data limitations and the fact that the modeling study encompassed less than 1,000 feet (305 meters) of the western plume's front made calibration of the historical plume behavior impossible. Therefore, the transport model was utilized to evaluate the characteristics of the plume within the bedrock valley sand and gravel deposits using the present distribution of contaminant as initial conditions and using the model to predict future distribution of the plume front. Although the model simulation of the present plume front was not calibrated, a range of values for transport parameters was simulated to test the sensitivity of plume migration to each parameter. These parameters included bedrock and sand and gravel hydraulic conductivity, longitudinal and transverse dispersivity, and effective porosity.

The contaminant source in the transport model was simulated by assigning a constant concentration in nodal cells within the central northeastern portion of the model, within the extent of the plume as shown in field-based contours of concentration (Figure 3-1). The plume extent is defined by the contour at which ground-water impacts would be non-detectable by current analytical technology. Simulations were run with and without

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degradation. Due to the similarities in physical and chemical processes for PCE and trichloroethylene (TCE), which are the dominant VOC compounds in ground water within the modeled area at the RHL site, only PCE was simulated in the transport model. Of the two compounds, PCE occurs at the higher concentration and has lower concentration standards for protection of public health (1 part per billion [ppb] Enforcement Standard [ES] and 0.1 ppb Preventive Action Limit [PAL]), as defined by Chapter NR140 Wisconsin Administrative Code.

For this study, the principal input parameters required to run MODFLOW at steady-state were hydraulic conductivity and the top and bottom elevations of the bedrock/sand and gravel aquifer. Option 3 in MODFLOW was used to define the layer type which was simulated as confined/unconfined. In this case, the transmissivity of the layer can vary and is calculated from the saturated thickness and hydraulic conductivity. This option was chosen in the event that the model was used to simulate dewatering conditions for a ground-water recovery system. For pumping simulations (transient conditions), the data required include confined storage coefficients and specific yields.

Input required of the MT3D transport model are the flow model heads and locations and flow rates of sinks/sources as solved by the flow model, along with data input described in the MT3D documentation on pages 6-10 through 6-30 in Appendix A. Among the more important parameters required in this study for each cell are the effective porosity of the medium, the boundary array for the concentration field, the longitudinal and transverse dispersivity arrays, and the first-order rate constant for the dissolved phase for degradation simulations.

The transport simulations utilized the advection, dispersion, sink and source mixing, and chemical reaction options in MT3D. This modeling study uses the hybrid method of characteristics scheme for the advection solution. In addition, the fourth-order Runge-Kutta algorithm is selected for particle tracking in sink/source cells and cells adjacent to sinks/sources, while the first-order Euler algorithm is used for cells elsewhere. The mixed Eulerian-Lagrangian method used in MT3D is virtually free of numerical dispersion, and is

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capable of handling the entire range of Peclet numbers from 0 to ∞ (Zheng, 1990). The Peclet number is a measure of the degree of advection domination. Finally, a fixed pattern of nine particles per cell is used for initial placement of moving particles.

3.3.1 Determination of Hydraulic Properties

The similarity between the hydraulic conductivities of the sand and gravel and the bedrock aquifers and the absence of significant vertical gradients observed during earlier studies (HSI, June, 1991) suggests that the aquifers act hydraulically as a single unit. Therefore, simulation of the bedrock valley as one layer means that parameter values in the vertical dimension are integrated into a single value at any given location. Hence, a composite hydraulic conductivity for each nodal cell was determined.

Based on monitor well boring logs, the greatest difference between the potentiometric surface of the sand and gravel aquifer and its top elevation within the model area of interest is several tens of feet. To avoid interpolating a top elevation for the sand and gravel unit, the elevation of the potentiometric surface was assumed to represent the top of the sand and gravel aquifer. This assumption had negligible effects on individual cell transmissivity calculations considering the average total saturated thickness of the model is greater than 230 feet.

To calculate composite conductivities, a series of steps involving hand contouring and computer database manipulation was required. Based on measured hydraulic heads from sand and gravel screened intervals at P-40, P-31, P-30, and P-41, a potentiometric surface map was interpolated by hand across the entire model grid (Figure 3-2). The observed head map in Figure 3-2, and all following maps, show conditions only within the area of plume migration. This area encompasses the 36 columns and 20 rows of regular-spaced nodes that are 100 feet (30 meters) square and are contained within the central portion of the grid (Figure 3-1). Choosing to show only regular-spaced nodes also facilitated the transfer of model output to the contouring program Surfer (Golden Software, 1990) which accurately represents only data that is regularly-spaced. Irregularly-spaced data can be entered into

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Surfer, but some corruption of data is possible. Furthermore, no field data were available to represent conditions accurately outside of the regularly-spaced node cells. Data from the above-named monitor wells were extrapolated to these areas. These areas were added to the grid to keep the shorter model boundaries at a distance from the plume so they would not affect transport solutions in the area of interest. The hydraulic conditions in these areas did not affect the transport simulations. The measured/interpolated heads were then subtracted from a uniform model base elevation of 658 feet to determine a saturated thickness value for each cell. The 658-foot elevation is based on the elevation of the bedrock surface at P-30, and is assumed to be measured where the thickness of sand and gravel deposits is greatest in this section of valley. This elevation is below the vertical extent of impacted ground water observed in the field investigation.

The next step was to determine the individual saturated thicknesses of sand and gravel and bedrock within each cell. Based on the drilling logs for P-40, P-31, P-30, P-39, and P-41, a contour map of sand and gravel thickness was interpolated by hand for the entire model grid. The highest topographic elevations within the grid and/or the cells where the potentiometric surface occurred in bedrock were designated as zero sand and gravel thickness (Figure 3-3). In general, the bedrock valley geometry detailed by the cross-sectional profile of P-40, P-31, P-30, and P-39 (HSI, June, 1991, Plates III and VII) was incorporated throughout the entire valley encompassed within the model. The measured/interpolated sand and gravel thickness was subtracted from the cell's potentiometric surface elevation to determine a sand and gravel saturated thickness. The base 658-foot elevation was then subtracted from the bottom elevation of the sand and gravel to determine the bedrock saturated thickness. Where sand and gravel was designated as zero thickness (Figure 3-3), the base elevation was subtracted from the potentiometric surface elevation to determine a bedrock saturated thickness.

After the saturated thicknesses for sand and gravel and bedrock were calculated for each cell, an average hydraulic conductivity for each unit was multiplied by the relevant thickness to determine a separate transmissivity for sand and gravel and for bedrock. The average hydraulic conductivity for sand and gravel deposits was 4.2 x 10⁻⁴ ft/sec (1.3 x 10⁻² cm/sec),

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and is an average of seven slug tests in sand and sand and gravel from HSI's earlier report (HSI, June, 1991). This value also lies within the range of sand and gravel conductivities reported in numerous sources.

The average bedrock hydraulic conductivity used for the above calculations was 8.3×10^{-5} ft/sec (2.5×10^{-3} cm/sec), and is an average of two slug tests in sandstone and dolomite in HSI's earlier report (HSI, June, 1991) and information from seven private wells in sandstone and dolomite (Muldoon, 1991) in the surrounding model area in which hydraulic conductivities were calculated from specific capacity data using the program TGUESS (Bradbury and Rothschild, 1985). The average value used for bedrock conductivity also agrees closely with those reported in McLeod (1975) and Cline (1965) for Upper Cambrian sandstones and dolomites in the region. However, it is recognized that hydraulic conductivity in bedrock may be higher locally due to fractures.

Table 3-1 shows hydraulic conductivity estimates used for calculating average values for model input. In cells where two separate transmissivities were calculated, a composite transmissivity was calculated from the average of the two. This composite transmissivity (Figure 3-4) was then divided by the total cell saturated thickness to determine a composite hydraulic conductivity which was entered into MODFLOW's Block-Centered Flow Package. The Basic, Strongly-Implicit Procedure and Output Control Packages were also used in the flow model. The input files for these packages are found in Appendix B1.

3.4 Representation of Model Input and Output

Because interpolation of hydraulic head and sand and gravel thickness for each cell within the model was done by hand, a geostatistical method for estimating data between measured locations, such as kriging, was not used. Although kriging is an accurate and popular geostatistical tool for data interpolation, the task of hand estimating 1,000 values for each of the above parameters was considered a worthwhile effort to maintain an optimal degree of control over the geometry of the bedrock valley unconsolidated deposits to be modeled

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and the head field which was critical to the gradients and flow velocities that were input to the transport model.

HSI's data post-processing program for the MODFLOW code reads an unformatted file containing the hydraulic head output, and writes a new file in a data format that can be read by Surfer (Golden Software, 1990) to generate a grid that can be used to develop a contour map of the study area's potentiometric surface. This process was used to interpret the changes in the head field with various aquifer parameter changes, and facilitated the flow model calibration process.

Likewise, the data post-processing program used in MT3D for ground-water concentration can generate grid-formatted files that Surfer (Golden Software, 1990) reads to produce contour maps. There is also the option of producing post-processing files for any portion of the model grid the user specifies. In this study, the model grid is designed to encompass the entire plume front within the regularly-spaced nodes (columns 8 through 43; Figure 3-1). Only this area is utilized in MT3D's post-processor and is transferred (as grid-formatted files) to Surfer which is designed primarily for regularly-spaced data.

3.5 Flow Model Calibration

Aquifer characterization consists of measuring head and describing the spatial and temporal variability in parameters such as hydraulic conductivity and effective porosity. The uncertainties associated with modeling results are caused by measurement errors, uneven distribution and number of data, simplifying assumptions incorporated into the conceptual model of the real aquifer system, and scaling errors caused by interpolation of field data to the model grid. Successful modeling requires understanding how to relate limited parameter values measured in the field for large-scale, heterogeneous, transient ground-water systems to the model. The calibration process is a critical check on the mathematical simulation of a ground-water system. A calibrated model reproduces data measured in the field given a set of hydrogeologic and boundary conditions and acceptable prediction criteria. Calibration is achieved by varying the least known hydraulic parameters within a pre-

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determined reasonable range until the simulated results match calibration targets within the pre-determined calibration criterion.

In this investigation, the model was considered calibrated when the difference between a measured/interpolated and simulated head was equal to or less than the head drop across the cell (Table 3-2). In this study, there are only four measured head locations. All observed/interpolated heads input to the model were taken from the interpolated potentiometric surface map. Therefore, each node was considered to be a calibration target. The smallest difference between a measured and simulated head is 0.01 feet (0.003 meters) at P-30I, while the largest difference of 0.18 feet (0.05 meters) is at P-40. Heads were assumed to represent steady-state conditions.

The root mean squared error (RMS) is an average measure of a calibration, or the goodness of fit between measured and modeled heads. RMS error is calculated by squaring the differences between simulated and observed heads, and then taking the square root of the mean of those squares for all the calibration targets. Ideally, the RMS error should equal zero, meaning a perfect fit, or at least be very small. For the RHL model, the RMS error for all cells is 0.07 feet (0.02 meters). The RMS error for measured locations is 0.13 feet (0.04 meters). The RMS error for all cells is less than the average head drop across all cells (0.2 feet). Likewise, the RMS error for measured locations is less than the average head drop across cells containing measured locations (0.15 feet). The RMS errors indicate a reasonably good model calibration and are considered acceptable because they are lower than the pre-determined calibration criteria discussed above (head drop across cells). Another criterion used as an average measure of a calibration is the ratio of the RMS error and the total head drop across the model. There is no general rule of thumb, but this value should also be small. The ratio of the RMS error for all cells and the average head drop across the model (approximately 3 feet) is 0.02 feet (0.006 meters).

The water budget for the calibrated flow model is balanced with a 0.00% discrepancy between inflows and outflows (Appendix C.1). A sensitivity analysis of the flow model was not performed because no information is available on regional ground-water fluxes into or

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out of the modeled area. Furthermore, a range of hydraulic conductivities was used in the transport simulations. Hydraulic conductivity input to the flow model (Table 3-3), as well as saturated thicknesses of bedrock/sand and gravel, remained unchanged during the calibration process. Only specified head boundaries on each side of the model were adjusted until a reasonable approximation of measured heads was achieved. Figure 3-5 compares the observed potentiometric surface with the model-calibrated head field. The same general ground-water flow pattern is represented for both conditions.

HSI's earlier report on the RHL site (HSI, June, 1991) estimated the velocity of ground water in bedrock downgradient of the RHL at 1.3×10^{-6} ft/sec (4.0×10^{-5} cm/sec). Ground-water velocity within sand and gravel deposits was estimated at 2.8×10^{-6} ft/sec (8.5×10^{-5} cm/sec). These estimates assumed a porosity of 10% and 30% (Freeze and Cherry, 1979) for bedrock and sand and gravel, respectively. Model-calibrated inflow velocities for bedrock ranged between 1.8×10^{-7} ft/sec and 5.3×10^{-7} ft/sec (5.5×10^{-6} cm/sec and 1.6×10^{-5} cm/sec). Inflow velocities for sand and gravel ranged between 1.4×10^{-7} ft/sec and 4.7×10^{-7} ft/sec (4.3×10^{-6} cm/sec and 1.4×10^{-5} cm/sec).

3.6 Model Simulation of Plume

As explained in Section 3.2, calibration of the plume's characteristics, such as shape and travel rate, was not possible. Hence, the present distribution of the plume was used as initial conditions; a range of values for transport parameters was evaluated during prediction runs of plume migration. The locations where point sources were simulated in the model are shown in Figure 3-6. A constant contaminant source of 12 parts per billion (ppb) was chosen to represent the plume concentration based on PCE analysis results from ground water sampled at wells immediately upgradient of the modeled plume area, and from ground water concentrations measured for PCE in P-40 and P-31 (Table 3-4) which are located at the leading edge of the modeled plume. In some simulations, it was assumed that the source of the contaminant is removed. In these simulations, point sources were changed to variable (active) concentrations during prediction runs so that concentrations already present within the aquifer eventually could be dissipated.

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Horizontal longitudinal dispersivity (a_L) values ranging from 10 to 50 feet were used during transport simulations for cells where saturated sand and gravel deposits are present (Figure 3-3). Simulated bedrock a_L ranged from 3 to 17 feet in those node cells where no saturated unconsolidated deposits are present. Values for horizontal transverse dispersivity (a_T) were maintained at approximately one-third the magnitude of the respective a_L. Sand and gravel a_T ranged from 3.3 to 16.5 feet, while bedrock a_T was simulated between 1.0 and 5.6 feet. The above horizontal and transverse dispersivities are taken from average field-measured or model-calibrated values reported in Gelhar et al. (1985) for alluvial sand and gravel and sandstone/dolomite bedrock. Values chosen as most representative of sand and gravel and bedrock a_L were 30 and 10 feet, respectively.

A range of commonly used effective porosities (n_e) was also used in simulating bedrock and sand and gravel properties. Sand and gravel n_e ranged between 20% and 30%, while bedrock n_e was between 3% and 10%. Values chosen as most representative for sand and gravel and bedrock n_e were 25% and 5%, respectively (Freeze and Cherry, 1979; Fetter, 1980; Domenico and Schwartz, 1990).

Organic contaminants can be transformed into other compounds by numerous chemical and biological mechanisms. Most of the effects of these mechanisms in the ground-water zone are not well understood. The principal chemical reactions affecting organic contaminants in water are hydrolysis and oxidation (Mackay et al., 1985). As for biological reactions, microorganisms attached to solid particulates within the aquifer can transform organics in ground water under both aerobic and anaerobic conditions. The principal breakdown products of PCE are TCE, 1,2-dichloroethylene (1,2-DCE), and vinyl chloride. Vinyl chloride cannot be transformed further under most natural conditions (Mackay et al., 1985).

At the RHL site, ground-water analyses indicate the possibility of degradation (meant here to include chemical and biological reactions) occurring south of the landfill within sand and gravel deposits because vinyl chloride has been detected in ground water. There is also the possibility of a source of vinyl chloride within the landfill; however, there is no evidence to support this. West of the landfill and in the modeled plume area, TCE and 1,2-DCE have

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been detected but vinyl chloride has not. In addition, PCE concentrations (Table 3-4) as well as TCE and 1,2-DCE (Table 3-5) have remained fairly constant over the past year or more in wells P-40 and P-31, and in two private wells upgradient from the modeled area.

It should be noted that the potential exists for vinyl chloride to occur at the RHL site, and that vinyl chloride has the lowest Public Health Groundwater Quality Standard (NR140) compared to PCE and other degradation products. The NR140 ES and PAL for vinyl chloride are 0.2 ppb and 0.0015 ppb, respectively. Therefore, compounds other than PCE may represent public health concerns at lower concentration and over shorter arrival times at receptors than modeled herein.

Although recent research (Roberts et al., 1986) has shown the long-term behavior (over two years) of PCE in a sand aquifer was to conserve total mass, some degradation is most likely occurring west of the RHL site. Published values for PCE half-life range from 230 days to 34 days (Olsen and Davis, 1990). A recently published handbook of environmental degradation rates (Howard et al., 1991) gives a range for PCE half-life in ground water of 730 to 365 days. Modeling a high degradation rate may underestimate plume migration, while a slow rate could overestimate movement of contaminants across the valley. Because of the uncertainty in degradation rate for this study, an intermediate rate of 230 days was simulated as well as scenarios using a slower 730-day half-life and no degradation. A 230-day half-life equates to a first order rate constant of 3.4×10^{-8} sec^{-1} ($^{0.693}$/half-life) which is entered into the chemical reaction package of MT3D. Only one value for degradation can be entered into the transport model. No retardation of solute by way of sorption was modeled due to the typically low organic matter content of sand and gravel, and to make conservative predictions of plume migration.

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4.0 INTERPRETATION OF MODEL RESULTS

4.1 Overview

The results of a sensitivity analysis to evaluate the effect of changing values of model input parameters showed the plume's migration to be most affected by hydraulic conductivity and degradation rate. The parameters found to have the least effect on plume movement were dispersivity and effective porosity. Furthermore, increasing the concentration source to 100 ppb had negligible effects on the migration rate or shape of the plume as compared to a 12 ppb concentration source.

When simulating those conditions judged to be most representative of the RHL site, model results show that after 5 years the plume is at equilibrium with dilution, dispersion, and degradation processes, and that further migration of PCE across the bedrock valley toward private residences in the Deer Run Subdivision is unlikely subject to uncertainties in model parameters. Simulations from the most conservative modeled scenario, although not considered representative of the real ground-water flow system, show PCE concentrations over 1 ppb arriving at P-30 after 2 years, at the closest private residence after 4 years, and at P-41 after 9 years. Simulations of representative conditions with the source of contaminants removed show that the presently existing PCE concentrations within the valley are non-detectable after approximately 2 years.

Evaluation of the routine monitoring strategy using the most conservative modeled scenario suggests that a sentry well should be installed near the middle of the bedrock valley in Figure 4-39. Monitor well sampling could be scheduled on semi-annual or annual intervals according to PCE arrival times predicted by the model under the conservative scenario.

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4.2 Evaluation of Plume Migration

4.2.1 Sensitivity Analyses

Sensitivity analyses were conducted to evaluate the plume's migration under various assumptions of hydraulic conductivity, longitudinal and transverse dispersivity, effective porosity, and whether PCE degradation occurs. The following sensitivity simulations were made to evaluate the significance of input parameters, and may not necessarily reflect conditions thought to be most representative of actual field conditions.

Results show the plume's migration to be most affected by hydraulic conductivity and degradation. The concentration contour map shown in Figure 4-1 shows results for the base case simulation. As stated in Section 3-6 and Section 4.2.2, representative values for sand and gravel and bedrock longitudinal dispersivity were estimated to be 30 and 10 feet, respectively, while porosities of 25% and 5% were simulated for sand and gravel and bedrock, respectively. These values are used in Figure 4-1. Figure 4-2 shows the results with degradation and increasing hydraulic conductivity uniformly by one order of magnitude over the base case values. This increase in conductivity is analogous to increasing ground-water velocities uniformly by ten times. A more significant effect in the plume's movement is shown in Figures 4-3 and 4-4 when the same increase in conductivity is made, but no degradation is simulated. As shown in Figure 4-4, model results show the plume spreading across the valley after only 5 years of simulation time. The above simulations are made under the assumption of a constant source of PCE at a concentration of 12 ppb.

During sensitivity analyses, the parameters found to have the least effect on the plume's shape or migration are dispersivity and effective porosity. A higher dispersivity for sand and gravel and bedrock of 50 and 17 feet, respectively, were simulated with the same conductivity and degradation conditions as Figures 4-1 through 4-4. A comparison of Figures 4-5 through 4-8 with Figures 4-1 through 4-4 shows a negligible difference in plume shape.

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Likewise, a lower dispersivity for sand and gravel and bedrock of 10 and 3 feet, respectively, were simulated under the same conductivity and degradation conditions as Figures 4-1 through 4-4. A comparison of Figures 4-9 through 4-12 with those figures also shows a negligible difference in plume migration.

Additional sensitivity analyses were performed to evaluate changes in effective porosity while keeping other conditions the same as Figures 4-1 through 4-4. A decrease in sand and gravel and bedrock porosity to 20% and 3% was simulated in Figures 4-17 through 4-20. These results are similar to the dispersivity changes, i.e, there is a negligible effect on the plume's migration rate or shape.

Likewise, increases in effective porosity to 30% and 10% for sand and gravel and bedrock, respectively, (Figures 4-21 through 4-24) also indicate a negligible change in the plume when compared to Figures 4-1 through 4-4.

Further sensitivity analyses were conducted using a constant concentration source of 100 ppb. As shown by comparing Figures 4-13 through 4-16 with Figures 4-1 through 4-4, the increase in concentration does not significantly affect the migration rate or shape of the plume from results with a 12 ppb concentration source.

A final set of analyses was performed to evaluate the plume's characteristics assuming that the source of contaminants is removed and contaminants presently within the bedrock valley aquifer are allowed to dissipate. These predictions were made by changing the point concentration model cells from constant to variable in MT3D's Basic Transport Package. Results when degradation is simulated (Figures 4-25 and 4-26) show no concentrations greater than 1 ppb present after approximately 1.8 years of simulation time using base case hydraulic conductivities (Figure 4-25) and after approximately 2.2 years when conductivities are increased one order of magnitude (Figure 4-26). Concentrations of PCE are less than 1 ppb at P-30 and wells west of that location (Figures 4-25 and 4-26). Results without degradation and with base case conductivities show that concentrations are greater than 1 ppb at P-30 after about 22 years (Figure 4-27), at the closest Deer Run home after 45 years

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(Figure 4-28), and at P-41 after about 75 years (Figure 4-29). Simulating an order of magnitude change in conductivity results in detections over 1 ppb of PCE at P-30 in about 2.2 years (Figure 4-30), at the closest private residence after 4.2 years (Figure 4-31), and at P-41 after about 10 years (Figure 4-32). A summary of these prediction times is presented in Table 4-1.

Although not considered representative of degradation conditions at the study site for reasons stated in Section 3.6, the model results for plume migration in Figure 4-4 could be considered the most conservative modeled scenario. A conservative scenario, in this case, is meant to imply more rapid contaminant flow across the bedrock valley. The plume is predicted to extend across the valley after a period of 5 years when modeling an order of magnitude increase in hydraulic conductivity and no degradation of PCE. Although the assumption of no degradation taking place is unlikely, the results in Figure 4-4 provide important insight concerning the future placement of additional monitor wells and for the establishment of monitoring frequency (Section 4.3).

4.2.2 Prediction Uncertainties

As stated in Section 3.6, the longitudinal dispersivities considered most representative for sand and gravel and bedrock are 30 and 10 feet, respectively. There is great uncertainty over the selection of appropriate dispersivities, in general. In this model, however, results are not sensitive to the choice of dispersivity value. A 25% and 5% effective porosity was also chosen as most representative of sand and gravel and bedrock, respectively. In addition, degradation (or partial decomposition) processes are thought to occur in the modeled area of interest based on detections of TCE and 1,2-DCE which are PCE transformation by-products (Table 3-5). Because no ground-water remediation system is in place at the RHL, a constant source of contaminants can be assumed. However, the possibility of higher than measured hydraulic conductivity is likely due to fracture flow in bedrock, preferential migration pathways in gravel, and the phenomenon that hydraulic conductivities in unconsolidated deposits increase when the operational scale of measurement increases (Bradbury and Muldoon, 1990). Slug test measurements performed

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at the RHL site from the small area immediately surrounding a monitor-well screen could easily be too low by an order of magnitude when used to represent a larger scale.

The model results that incorporate the above conditions and thereby are judged to be most representative of the RHL model site are presented in Figures 4-1 and 4-2. Model predictions for both base case conductivities (Figure 4-1) and increased conductivities (Figure 4-2) indicate a steady-state condition exists after a simulation period of 5 years. Plume migration, shape, and predicted PCE concentrations at P-30 and P-41 remain virtually the same when using simulation times of 53 and 100 years (Figures 4-1a and 4-2a).

Chemical mass balances for Figures 4-1 and 4-2 are -11.2 and 1.9%, respectively (Appendix C.2). According to Konikow (1991, personal communication), the mass balance calculation for MOC is only an approximation of average nodal concentrations. The model calculations are based on particle concentrations and positions, and can be more accurate than the mass balance indicates. Because mass balance calculations average nodal concentrations, the balance errors can oscillate within +/-10% as particles move. For the MT3D transport model, which is based on MOC, mass balance errors up to 12% are not unreasonable (Zheng, 1991, personal communication).

The Peclet number (grid cell width/longitudinal dispersivity) ranges between 2 and 10 for all transport simulations, and equals approximately 3 for Figures 4-1 and 4-2. The Courant number, or the number of cells any particle is allowed to move in any direction in one transport step, equals 0.75 for all simulations. In general, the range of Courant numbers recommended in MT3D documentation is between 0.5 and 1.

Results using a slower, conservative estimate of 730 days for PCE half-life (Howard et al., 1991) show slightly more spreading of contaminant under base case hydraulic conductivity conditions (Figure 4-1b). When using this same slower rate and increased conductivities, simulations show significantly more spreading of PCE across the valley (Figure 4-2b) than that shown for conditions in Figure 4-2 when the intermediate 230 day half-life is simulated. Detections of PCE over 1 ppb at well P-30 after 3 years and at the nearest private well after

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approximately 5 years are also indicated (Table 4-1). Results for this range of PCE half-life are presented due to the uncertainty in this chemical's degradation rate under various aquifer conditions existing within the study area..

The simulations in Figures 4-1 and 4-2 indicate that after 5 years the plume is at equilibrium with dilution, dispersion, and degradation processes, and that further migration of PCE across the bedrock valley toward private residences in the Deer Run Subdivision is unlikely. Although the above conclusions are judged as the most representative predictions of plume migration at the RHL, any remedial or monitoring decisions based on this report should account for the reality that model results reflect the constraints and assumptions that are present concerning the numerical representation of the real field system and its hydraulic boundaries at the site, particularly the assumption of the degradation rate. The model results should not be construed as conclusive that downgradient wells will not be impacted in the future.

Although the absence of degradation of PCE is considered unlikely, simulations performed without degradation under representative conditions predicted arrival times of concentrations over 1 ppb PCE at P-30 at approximately 2.1 (Figure 4-34) and 20 years (Figure 4-33), at the closest private residence at 4.1 (Figure 4-35) and 40 years (Figure 4-36), and at P-41 at 9 (Figure 4-37) and 100 years (Figure 4-38). These time predictions are also summarized in Table 4-1.

As stated in Section 4.2.1, model simulations using increased hydraulic conductivities and no degradation (Figure 4-4) could be considered a more protective or conservative scenario. As shown in Table 4-1, model predictions of PCE concentrations greater than 1 ppb are predicted to arrive at P-30 after 2.1 years, at the closest Deer Run residence after 4.1 years, and at P-41 after 9 years.

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4.3 Monitoring Strategy Implications

Model predictions of plume migration have important implications concerning the possible placement of additional monitor wells and the long-term monitoring frequency of existing wells. Sentry wells could be placed in areas identified by the model as possible preferential pathways for plume migration. Monitor well sampling frequency should also take into consideration the predicted arrival times of PCE at specific locations within the bedrock valley.

Probably the best overall conditions for evaluating the future monitoring strategy in the model area are those that resulted in the plume configuration shown in Figure 4-4. This prediction was previously described as a conservative scenario whereby the plume traveled across the valley after approximately 5 years when simulating increased conductivities and no degradation. Based on this predicted plume migration, an additional sentry well should be considered near the location indicated in Figure 4-39. This location considers the westerly migration of the plume, and could provide early indication that contaminants have reached the middle of the bedrock valley. The location of this sentry well is also near the leading edge of the predicted plume after 5 years shown in Figure 4-2, which was stated previously as one set of conditions believed to be representative of the model site.

Based also on the conservative scenarios shown in Figure 4-4 and Table 4-1, monitoring frequency could be scheduled on semi-annual or annual intervals as PCE detections greater than 1 ppb are predicted to arrive at P-30 after 2 years and at the closest private residence in Deer Run Subdivision after 4 years. Any scheduled sampling event should include: 1) P-30, 2) the sentry well, if constructed, and 3) the closest Deer Run private well(s).

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5.0 CONCLUSIONS AND RECOMMENDATIONS

The modeling study resulted in the following conclusions:

♦ The interface between bedrock and valley deposits has significant effects on contaminant plume migration.

♦ Model predictions on plume migration were most sensitive to changes in hydraulic conductivity and whether degradation was simulated, while the least sensitive parameters analyzed were dispersivity and effective porosity;

♦ Model parameters judged to be most representative of the study site include: 1) 30 and 10 feet for sand and gravel and bedrock longitudinal dispersivity, respectively, and 25% and 5% for effective porosity of sand and gravel and bedrock, respectively; 2) a 12 ppb PCE concentration source with a degradation half-life rate of 230 days; and 3) base case hydraulic conductivities ranging between 3.9×10^{-5} ft/sec and 2.0×10^{-4} ft/sec.

♦ Under assumptions which are believed to be reasonable and representative of site conditions, the plume reaches an equilibrium condition after a period of approximately 5 years due to dispersion, dilution, and degradation processes.

♦ Although a "no degradation" scenario is considered unlikely, model results when simulating no degradation with both base case and higher conductivities show PCE concentrations over 1 ppb arriving at monitor well P-30 after 2.1 and 20 years, respectively, at the closest Deer Run subdivision home after 4.1 and 40 years, respectively, and at monitor well P-41 after 9 and 100 years, respectively.

♦ Model results using a slower degradation half-life rate of 730 days (the longest degradation rate found in the referenced literature) show the plume reaching an equilibrium condition after 7.5 and 7.2 years when base case and higher

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conductivities are simulated, respectively. PCE detections over 1 ppb are only predicted at monitor well P-30 and the closest Deer Run private home after 2.5 and 5 years, respectively, when modeling higher conductivities.

♦ An increase in source concentration has negligible effects on plume shape or travel rate;

♦ A conservative scenario simulating higher conductivities and no degradation predicts PCE concentrations over 1 ppb arriving at monitor well P-30 after 2 years, at the closest private home in Deer Run Subdivision after 4 years, and at monitor well P-41 after 9 years when assuming a constant 12 ppb source of contaminant;

♦ Simulations of representative conditions after the source of contaminants is removed suggest PCE concentrations within the valley would be non-detectable after approximately 2 years; and

♦ While model results suggest that migration of PCE across the valley is unlikely, the predictions for plume behavior cannot be considered conclusive due to the inherent uncertainties in model input parameters such as the rate of PCE degradation. Ground-water analyses indicate the presence of biodegradation and/or transformation by-products of PCE within the model area. However, the rate of this decay can only be estimated.

Based on the above, we make the following recommendations:

♦ A sentry well should be constructed near the location shown in Figure 4-39. Vertical profiling of ground water is suggested during well installation to determine if VOCs are already present and to determine an appropriate well depth.

♦ Monitor well sampling should be scheduled on a semi-annual frequency for the next 5 years and samples should be analyzed for VOCs using U.S. Environmental

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Protection Agency Method 502.2. This method represents the lowest available detection limit for PCE and its degradation by-products. If appropriate, sampling frequency could be reduced to annually after the 5-year period.

♦ Each sampling event, at a minimum, should include: 1) monitor well P-30, 2) the recommended sentry well, and 3) the closest private well(s) to the model area in Deer Run Subdivision.

♦ In the future event that PCE or other contaminants are detected in the above wells, the transport model should be recalibrated and/or used to simulate new conditions based on the field observations existing at that time.

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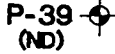
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PROJECT: 148E13673   DATE: 03/16/92

WI DEPT. OF NATURAL RESOURCES
REFUSE HIDEAWAY LANDFILL
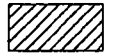
TOTAL VOCs AND
MODEL AREA

DRAWING NO.: 1367-13   FIGURE: 2-1

	Hydro-Search, Inc.	WI DEPT. OF NATURAL RESOURCES REFUSE HIDEAWAY LANDFILL
	HYDROLOGISTS GEOLOGISTS ENGINEERS	January 1991 TETRACHLOROETHENE ISOCONCENTRATION MAP AND MODEL GRID DISCRETIZATION
	Reno Denver Milwaukee Irvine	
PROJECT: 148E13673	DATE: 02/05/92	DRAWING NO.: 1367-15	FIGURE: 3-1
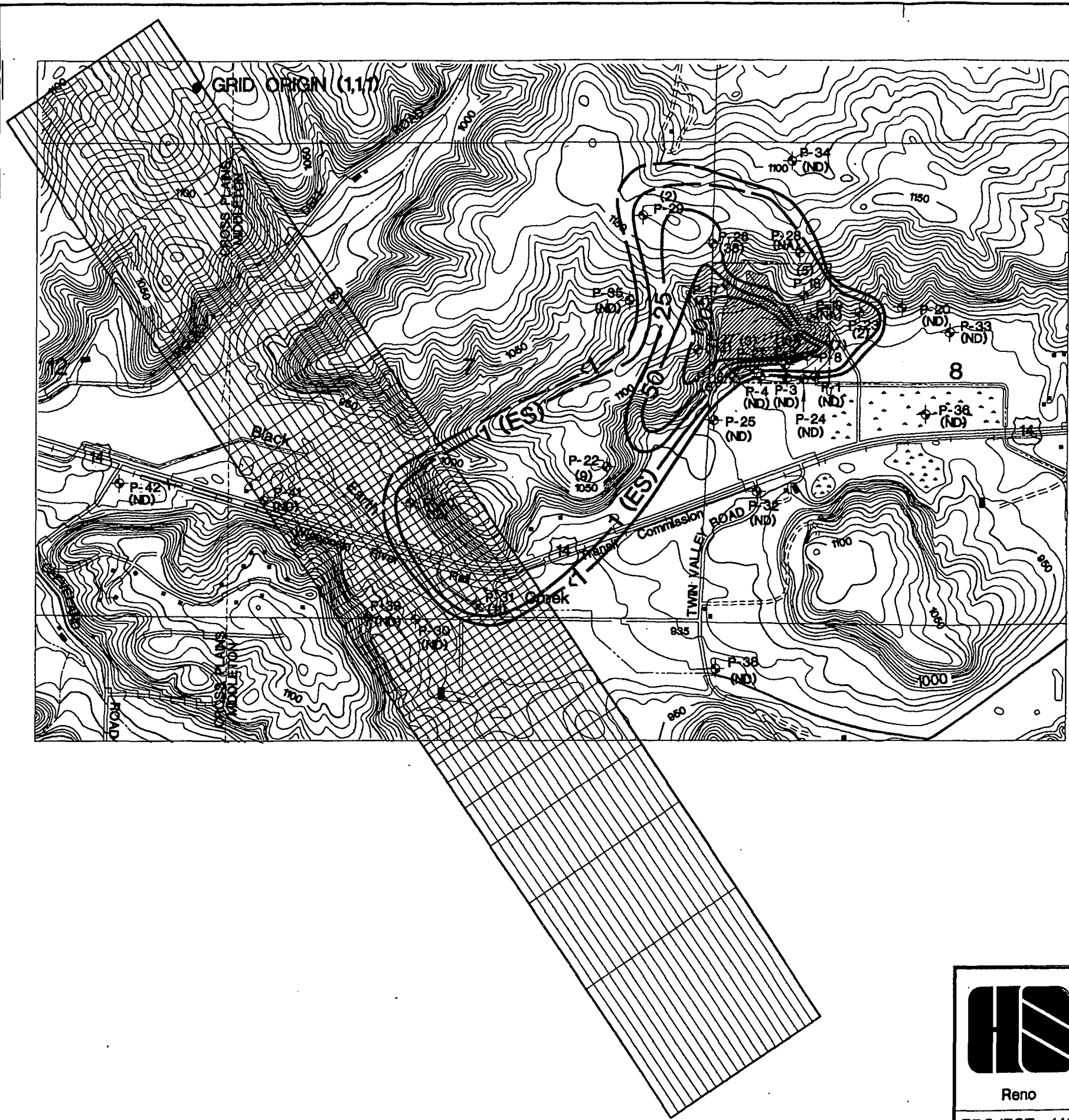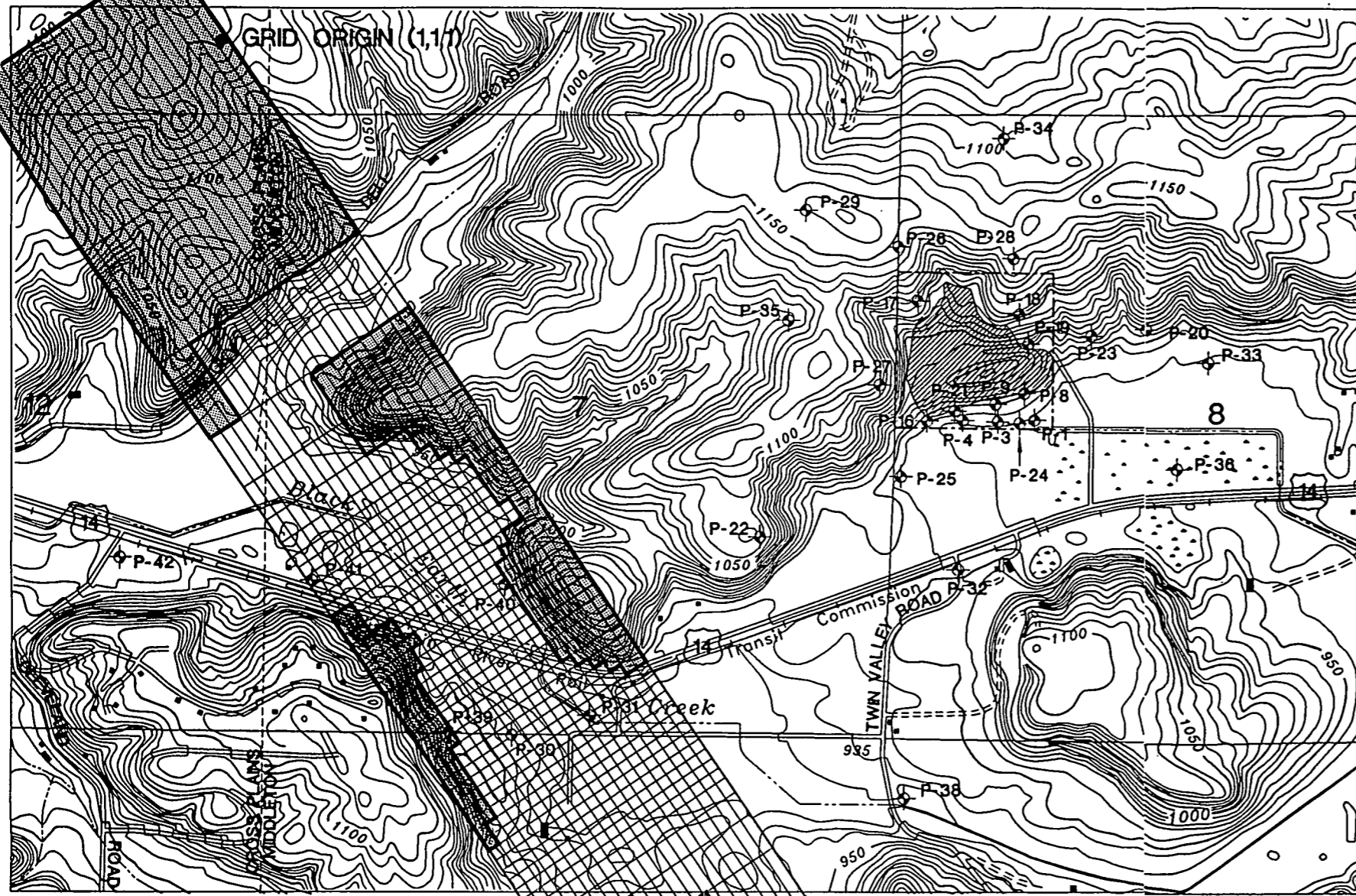
EXPLANATION

—·——·— REFUSE HIDEAWAY LANDFILL PROPERTY BOUNDARY

FILL LIMITS

P-39 -⊘- MONITOR WELL LOCATION, AND DESIGNATION

LOCATIONS WHERE SAND/GRAVEL THICKNESS IS ZERO

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0   2500

FEET
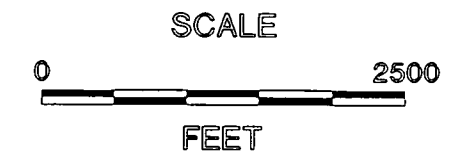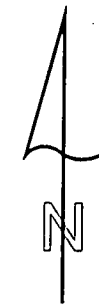
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REFUSE HIDEAWAY LANDFILL

LOCATIONS WHERE SAND/GRAVEL
THICKNESS IS ZERO IN MODEL

PROJECT: 148E13673 | DATE: 05/23/91 | DRAWING NO.: 1367-11 | FIGURE: 3-3

EXPLANATION

P-30 ⌀ MONITOR WELL

—0.045— TRANSMISSIVITY CONTOUR (ft^2/sec)

◆ closest Deer Run homes
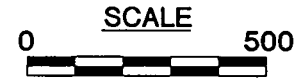
SCALE

0 ⎯⎯⎯⎯⎯⎯⎯ 500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

Hydro-Search, Inc.	WISCONSIN DEPT. OF NATURAL RESOURCES REFUSE HIDEAWAY LANDFILL
HYDROLOGISTS GEOLOGISTS ENGINEERS Reno Denver Milwaukee Irvine Sacramento	TRANSMISSIVITY OF BEDROCK/SAND & GRAVEL IN PLUME AREA

| PROJECT: 148E13673 | DATE: 1/21/92 | DRAWING NO.: 1367-t | FIGURE: 3-4 |

EXPLANATION

P-30 ⊕ MONITOR WELL

—906.2— POTENTIOMETRIC SURFACE CONTOUR
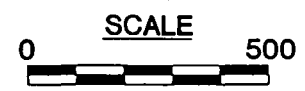
Topographic Contour Interval 10ft.
Datum is Mean Sea Level
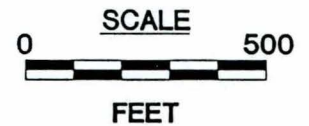
SCALE

0   500

FEET

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OBSERVED/INTERPOLATED
POTENTIOMETRIC SURFACE
IN PLUME AREA

PROJECT: 148E13673   DATE: 1/21/92   DRAWING NO.: 1367-kh1   FIGURE: 3-2

EXPLANATION

P-30 ⌀ MONITOR WELL

— 906.2 — OBSERVED POTENTIOMETRIC CONTOUR

— 906.2 — CALIBRATED POTENTIOMETRIC CONTOUR

■ ◆ closest Deer Run homes

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

SCALE
0   500

FEET

P-40
(906.13)

P-31
(906.48)

P-30
(905.85)

P-39

P-41
(903.80)

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HYDROLOGISTS GEOLOGISTS ENGINEERS Reno Denver Milwaukee Irvine Sacramento	COMPARISON OF OBSERVED/INTERPOLATED AND MODEL-CALIBRATED POTENTIOMETRIC SURFACE

| PROJECT: 148E13673 | DATE: 12/03/91 | DRAWING NO.: 1367-kch1 | FIGURE: 3-5 |

EXPLANATION

P-30 ϕ MONITOR WELL
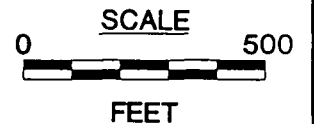
closest Deer Run homes

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

SCALE

0   500

FEET

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WISCONSIN DEPT. OF NATURAL RESOURCES
REFUSE HIDEAWAY LANDFILL

MODEL GRID LOCATIONS WHERE
POINT CONCENTRATION SOURCES
WERE SIMULATED

PROJECT: 148E13673   DATE: 12/03/91   DRAWING NO.:   1367-15   FIGURE: 3-6

closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb – constant source
Base K's

EXPLANATION

P-30 ◆ MONITOR WELL

—12.0—— ISOCONCENTRATION CONTOUR

SCALE

0 ————————— 500

FEET
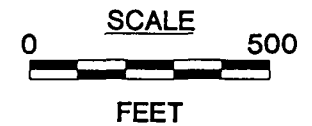
Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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PCE PLUME WITH
DEGRADATION AFTER 5 YEARS
(contour interval 2ppb)

| PROJECT: 148E13673 | DATE: 12/03/91 | DRAWING NO.: 1367-c2 | FIGURE: 4-1 |

P-40

P-31

P-30

P-39

P-41

Black

Earth

Creek

S.T.H. 14

■◆ closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb – constant source
Base K's

EXPLANATION

P-30-◆- MONITOR WELL

— 4.0 —— ISOCONCENTRATION CONTOUR

SCALE

0   500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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REFUSE HIDEAWAY LANDFILL

PCE PLUME WITH
DEGRADATION AFTER 100 YEARS
(contour interval 2ppb)

PROJECT: 148E13673	DATE: 12/03/91	DRAWING NO.: 1367-c2a	FIGURE: 4-1a

Map labels (within figure):

P-40 P-31 P-30 P-39 P-41

Black *Earth* *Creek* S.T.H. 14

■ ◆ closest Deer Run homes

1000 950 1050 12.0 8.0 4.0

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb – constant source
Base K's   730 day half-life

EXPLANATION

P-30 ◆ MONITOR WELL

—12.0—— ISOCONCENTRATION CONTOUR

SCALE

0 ──────── 500

FEET
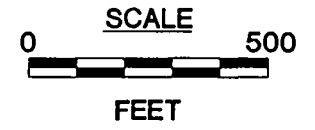
Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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**PCE PLUME WITH
DEGRADATION AFTER 5 YEARS**
(contour interval 2ppb)

PROJECT: 148E13673   DATE: 12/03/91   DRAWING NO.: 1367-c2b   FIGURE: 4-1b

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb - constant source
Base K's x10

EXPLANATION

P-30 ⟡ MONITOR WELL

— 4.0 — ISOCONCENTRATION CONTOUR

SCALE

0 _____ 500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

■ ◆ closest Deer Run homes

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REFUSE HIDEAWAY LANDFILL

**PCE PLUME WITH
DEGRADATION AFTER 5 YEARS**
(contour interval 2ppb)

PROJECT: 148E13673 | DATE: 12/03/91 | DRAWING NO.: 1367-C5 | FIGURE: 4-2

Map labels:
- 1000
- 950
- 1050
- 1000
- 950
- 12.0
- 8.0
- 4.0
- P-40
- 950
- P-31
- 12.0
- 8.0
- 4.0
- Earth
- Creek
- Black
- S.T.H. 14
- P-30
- 950
- P-39
- 1000
- 950
- P-41
- 1050
- 950
- ■ ◆ closest Deer Run homes
- N

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb – constant source
Base K's x10

EXPLANATION

P-30-� MONITOR WELL

— 4.0 — ISOCONCENTRATION CONTOUR

SCALE

0 ————————— 500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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REFUSE HIDEAWAY LANDFILL

**PCE PLUME WITH
DEGRADATION AFTER 53 YEARS
(contour interval 2ppb)**

PROJECT: 148E13673   DATE: 12/03/91   DRAWING NO.: 1367-c5a   FIGURE: 4-2a
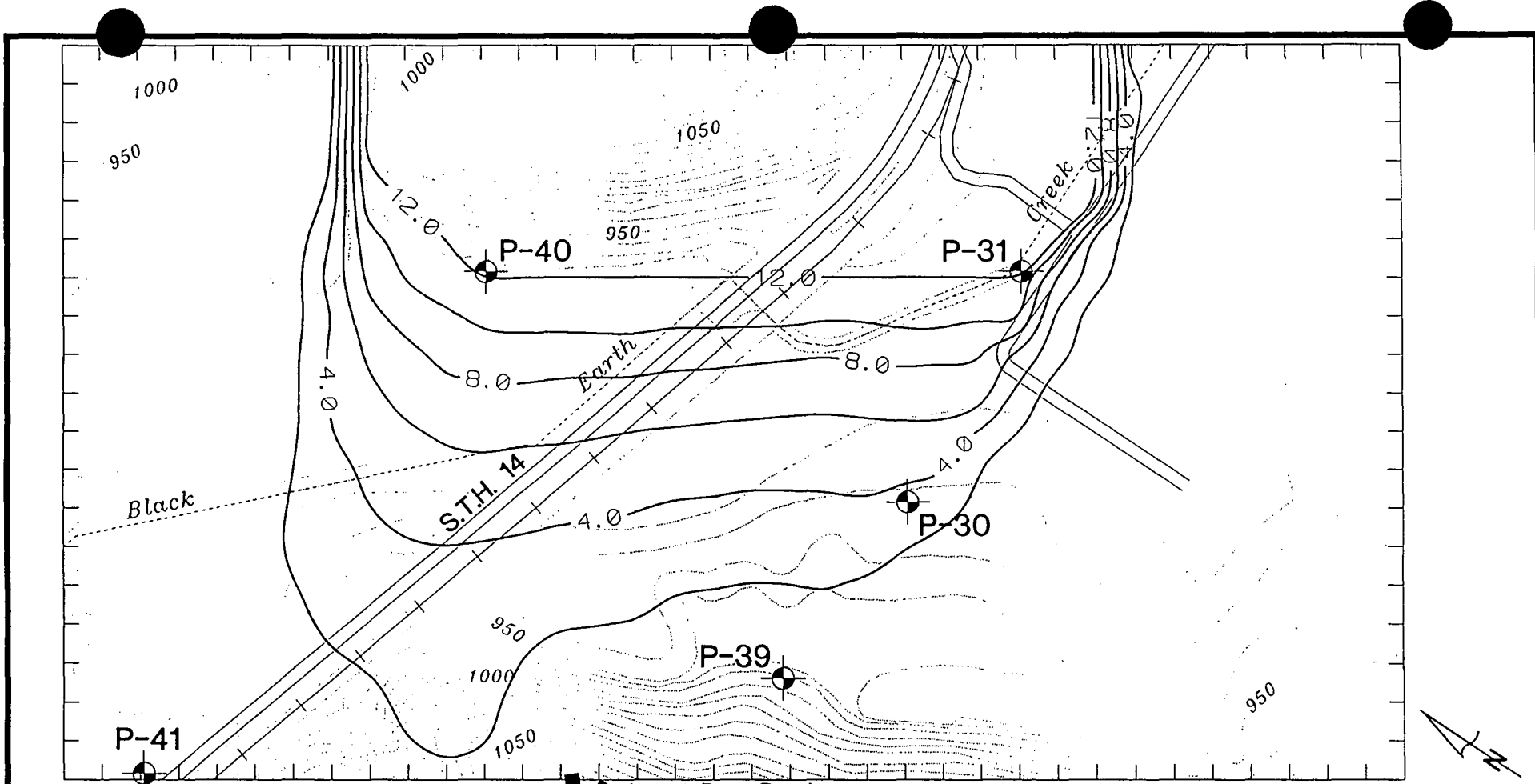
closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%
12ppb – constant source		
Base K's x10	730 Day half-life	

EXPLANATION
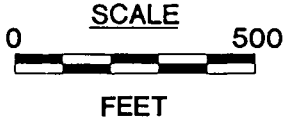
P-30-⬦- MONITOR WELL

— 4.0 — ISOCONCENTRATION CONTOUR

SCALE

0 ————————— 500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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REFUSE HIDEAWAY LANDFILL

PCE PLUME WITH DEGRADATION AFTER 5 YEARS
(contour interval 2ppb)

PROJECT: 148E13673   DATE: 12/03/91   DRAWING NO.: 1367-c5b   FIGURE: 4-2b

Map labels:
- 1000, 1050, 950 (topographic contours)
- P-40
- P-31
- P-30
- P-39
- P-41
- 12.0, 8.0, 4.0 (isoconcentration contours)
- Creek
- Earth
- Black
- S.T.H. 14
- closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb – constant source
Base K's

EXPLANATION

P-30 ⊕ MONITOR WELL

—12.0— ISOCONCENTRATION CONTOUR

SCALE

0 _____ 500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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PCE PLUME WITHOUT
DEGRADATION AFTER 5 YEARS
(contour interval 2ppb)

PROJECT: 148E13673   DATE: 12/03/91   DRAWING NO.: 1367-c3   FIGURE: 4-3

closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb - constant source
Base K's x10

EXPLANATION

P-30 ◆ MONITOR WELL

— 4.0 — ISOCONCENTRATION CONTOUR

SCALE

0 _____ 500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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PCE PLUME WITHOUT DEGRADATION AFTER 5 YEARS
(contour interval 2ppb)
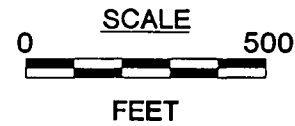
PROJECT: 148E13673   DATE: 12/03/91   DRAWING NO.: 1367-c4   FIGURE: 4-4

MODEL CONDITIONS

DISPERSIVITY	s/g	bedrock
DISPERSIVITY	50ft.	17ft.
EFFECTIVE POROSITY	25%	5%

12ppb - constant source
Base K's

EXPLANATION

P-30-⊕- MONITOR WELL

— 4.0 — ISOCONCENTRATION CONTOUR

SCALE

0   500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

closest Deer Run homes

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REFUSE HIDEAWAY LANDFILL

PCE PLUME WITH
DEGRADATION AFTER 5 YEARS
(contour interval 2ppb)

| PROJECT: 148E13673 | DATE: 12/03/91 | DRAWING NO.: 1367-c6 | FIGURE: 4-5 |

Map labels within the figure:

- 1000
- 950
- 1050
- 1050
- 950
- Creek
- P-40
- P-31
- 12.0
- 8.0
- 8.0
- 4.0
- 4.0
- 12.0
- Earth
- S.T.H. 14
- Black
- P-30
- 950
- 1000
- P-39
- P-41
- 1050
- 950
- ■◆ closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	50ft.	17ft.
EFFECTIVE POROSITY	25%	5%

12ppb - constant source
Base K's x10

EXPLANATION

P-30 ⟡ MONITOR WELL

— 4.0 — ISOCONCENTRATION CONTOUR

SCALE

0 _____ 500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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PCE PLUME WITH DEGRADATION AFTER 5 YEARS
(contour interval 2ppb)
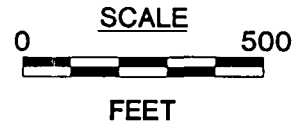
PROJECT: 148E13673	DATE: 12/03/91	DRAWING NO.: 1367-c8	FIGURE: 4-6

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	50ft.	17ft.
EFFECTIVE POROSITY	25%	5%

12ppb - constant source
Base K's

EXPLANATION

P-30 ⊕ MONITOR WELL

— 4.0 — ISOCONCENTRATION CONTOUR

■ ◆ closest Deer Run homes

SCALE

0 ————————— 500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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REFUSE HIDEAWAY LANDFILL

**PCE PLUME WITHOUT
DEGRADATION AFTER 5 YEARS**
(contour interval 2ppb)

PROJECT: 148E13673	DATE: 12/03/91	DRAWING NO.: 1367-c7	FIGURE: 4-7

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	50ft.	17ft.
EFFECTIVE POROSITY	25%	5%

12ppb – constant source
Base K's x10

EXPLANATION

P-30 ⬦ MONITOR WELL

— 4.0 — ISOCONCENTRATION CONTOUR

◼ ◆ closest Deer Run homes

SCALE

0 _____ 500

FEET
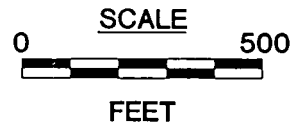
Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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**PCE PLUME WITHOUT
DEGRADATION AFTER 5 YEARS**
(contour interval 2ppb)

PROJECT: 148E13673	DATE: 12/03/91	DRAWING NO.: 1367-c9	FIGURE: 4-8
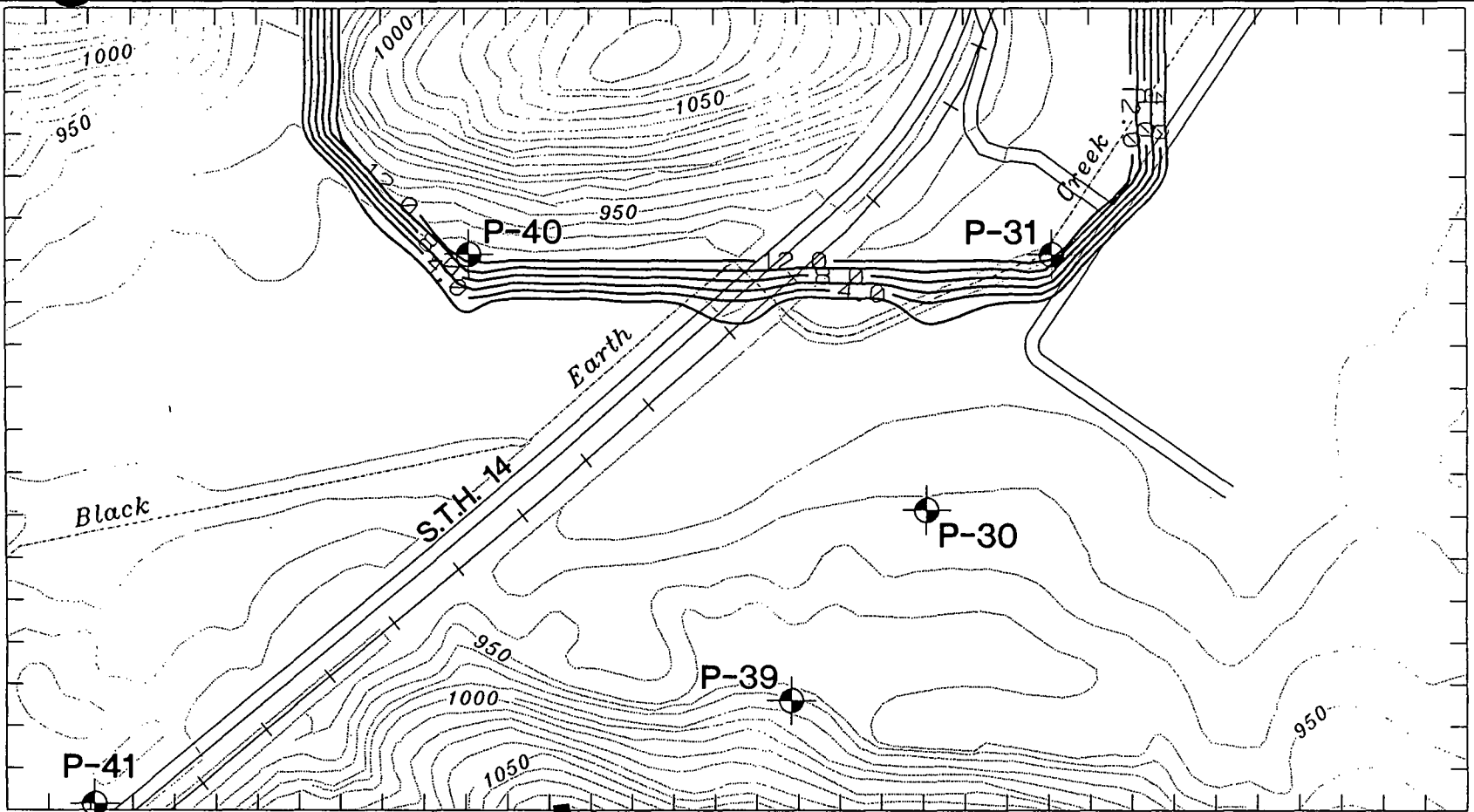
closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	10ft.	3ft.
EFFECTIVE POROSITY	25%	5%

12ppb - constant source
Base K's

EXPLANATION

P-30-⊕ MONITOR WELL

———— ISOCONCENTRATION CONTOUR
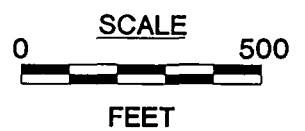
SCALE

0   500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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REFUSE HIDEAWAY LANDFILL

PCE PLUME WITH
DEGRADATION AFTER 5 YEARS
(contour interval 2ppb)

PROJECT: 148E13673	DATE: 12/03/91	DRAWING NO.: 1367-c10	FIGURE: 4-9

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	10ft.	3ft.
EFFECTIVE POROSITY	25%	5%

12ppb – constant source
Base K's x10

EXPLANATION

P-30-⊕ MONITOR WELL

—12.0—— ISOCONCENTRATION CONTOUR

SCALE

0   500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

closest Deer Run homes
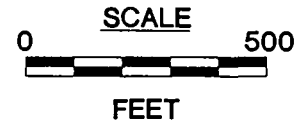
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REFUSE HIDEAWAY LANDFILL

PCE PLUME WITH
DEGRADATION AFTER 5 YEARS
(contour interval 2ppb)

PROJECT: 148E13673	DATE: 12/03/91	DRAWING NO.: 1367-c12	FIGURE: 4-10

closest Deer Run homes

MODEL CONDITIONS

DISPERSIVITY	s/g	bedrock
DISPERSIVITY	10ft.	3ft.
EFFECTIVE POROSITY	25%	5%

12ppb – constant source
Base K's

EXPLANATION

P-30-⬦— MONITOR WELL

—12.0—— ISOCONCENTRATION CONTOUR

SCALE

0   500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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PCE PLUME WITHOUT
DEGRADATION AFTER 5 YEARS
(contour interval 2ppb)

closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	10ft.	3ft.
EFFECTIVE POROSITY	25%	5%

12ppb – constant source
Base K's x10

EXPLANATION

P-30 ◆ MONITOR WELL

—12.0— ISOCONCENTRATION CONTOUR

SCALE

0   500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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**PCE PLUME WITHOUT
DEGRADATION AFTER 5 YEARS**
(contour interval 2ppb)

| PROJECT: 148E13673 | DATE: 12/03/91 | DRAWING NO.: 1367–c13 | FIGURE: 4-12 |

P-40

P-31

Creek

950

1000

1050

1000

950

Earth

S.T.H. 14

Black

P-30

P-39

950

1000

1050

950

P-41

■ ◆ closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

100ppb – constant source
Base K's

EXPLANATION

P-30-◆ MONITOR WELL

—40.0— ISOCONCENTRATION CONTOUR

SCALE

0   500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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PCE PLUME WITH
DEGRADATION AFTER 5 YEARS
(contour interval 20ppb)

PROJECT: 148E13673

DATE: 12/03/91
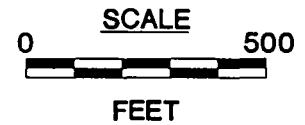
DRAWING NO.: 1367-c22

FIGURE: 4-13

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

100ppb – constant source
Base K's x10

EXPLANATION

P-30 ⊕ MONITOR WELL

—40.0—— ISOCONCENTRATION CONTOUR

SCALE

0 ————— 500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

◆ closest Deer Run homes

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REFUSE HIDEAWAY LANDFILL

**PCE PLUME WITH
DEGRADATION AFTER 5 YEARS**
(contour interval 20ppb)
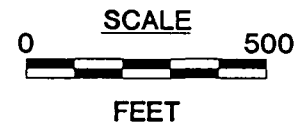
| PROJECT: 148E13673 | DATE: 12/03/91 | DRAWING NO.: 1367-c24 | FIGURE: 4-14 |

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

100ppb - constant source
Base K's

EXPLANATION

P-30-◆- MONITOR WELL

—40.0— ISOCONCENTRATION CONTOUR

■ ◆ closest Deer Run homes

SCALE

0   500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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REFUSE HIDEAWAY LANDFILL

PCE PLUME WITHOUT
DEGRADATION AFTER 5 YEARS
(contour interval 20ppb)
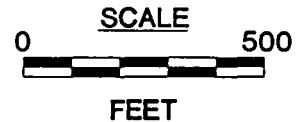
| PROJECT: 148E13673 | DATE: 12/03/91 | DRAWING NO.: 1367-c23 | FIGURE: 4-15 |

closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

100ppb – constant source
Base K's x10

EXPLANATION

P-30 �⬩ MONITOR WELL

—40.0— ISOCONCENTRATION CONTOUR

SCALE
0   500

FEET

Topographic Contour Interval 10ft.
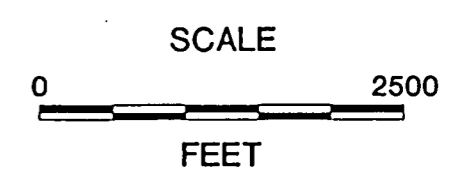Datum is Mean Sea Level

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WISCONSIN DEPT. OF NATURAL RESOURCES
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PCE PLUME WITHOUT
DEGRADATION AFTER 5 YEARS
(contour interval 20ppb)
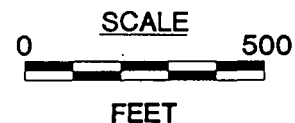
PROJECT: 148E13673	DATE: 12/03/91	DRAWING NO.: 1367-c25	FIGURE: 4-16

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	20%	3%

12ppb - constant source
Base K's

EXPLANATION

P-30 ⊕ MONITOR WELL

—12.0— ISOCONCENTRATION CONTOUR

■ ◆ closest Deer Run homes

SCALE

0 _____ 500

FEET
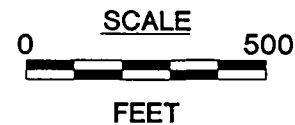
Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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PCE PLUME WITH
DEGRADATION AFTER 5 YEARS
(contour interval 2ppb)

PROJECT: 148E13673	DATE: 12/03/91	DRAWING NO.: 1367-c14	FIGURE: 4-17

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	20%	3%

12ppb - constant source
Base K's x10

EXPLANATION

P-30-⊕- MONITOR WELL

—12.0—— ISOCONCENTRATION CONTOUR

SCALE

0 _____ 500

FEET
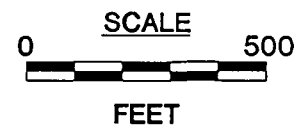
Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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**PCE PLUME WITH
DEGRADATION AFTER 5 YEARS**
(contour interval 2ppb)

| PROJECT: 148E13673 | DATE: 12/03/91 | DRAWING NO.: 1367-c16 | FIGURE: 4-18 |

P-40

P-31

P-30

P-39

P-41

Black

S.T.H.-14

Earth

Creek

■ ◆ closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	20%	3%

12ppb – constant source
Base K's

EXPLANATION

P-30 ⟡ MONITOR WELL

——12.0—— ISOCONCENTRATION CONTOUR

SCALE
0   500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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PCE PLUME WITHOUT
DEGRADATION AFTER 5 YEARS
(contour interval 2ppb)
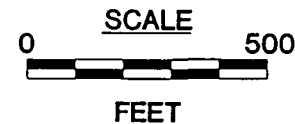
PROJECT: 148E13673	DATE: 12/03/91	DRAWING NO.: 1367-c15	FIGURE: 4-19

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	20%	3%

12ppb - constant source
Base K's x10

EXPLANATION

P-30-⬦- MONITOR WELL

—12.0— ISOCONCENTRATION CONTOUR

SCALE

0   500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

closest Deer Run homes
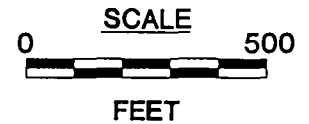
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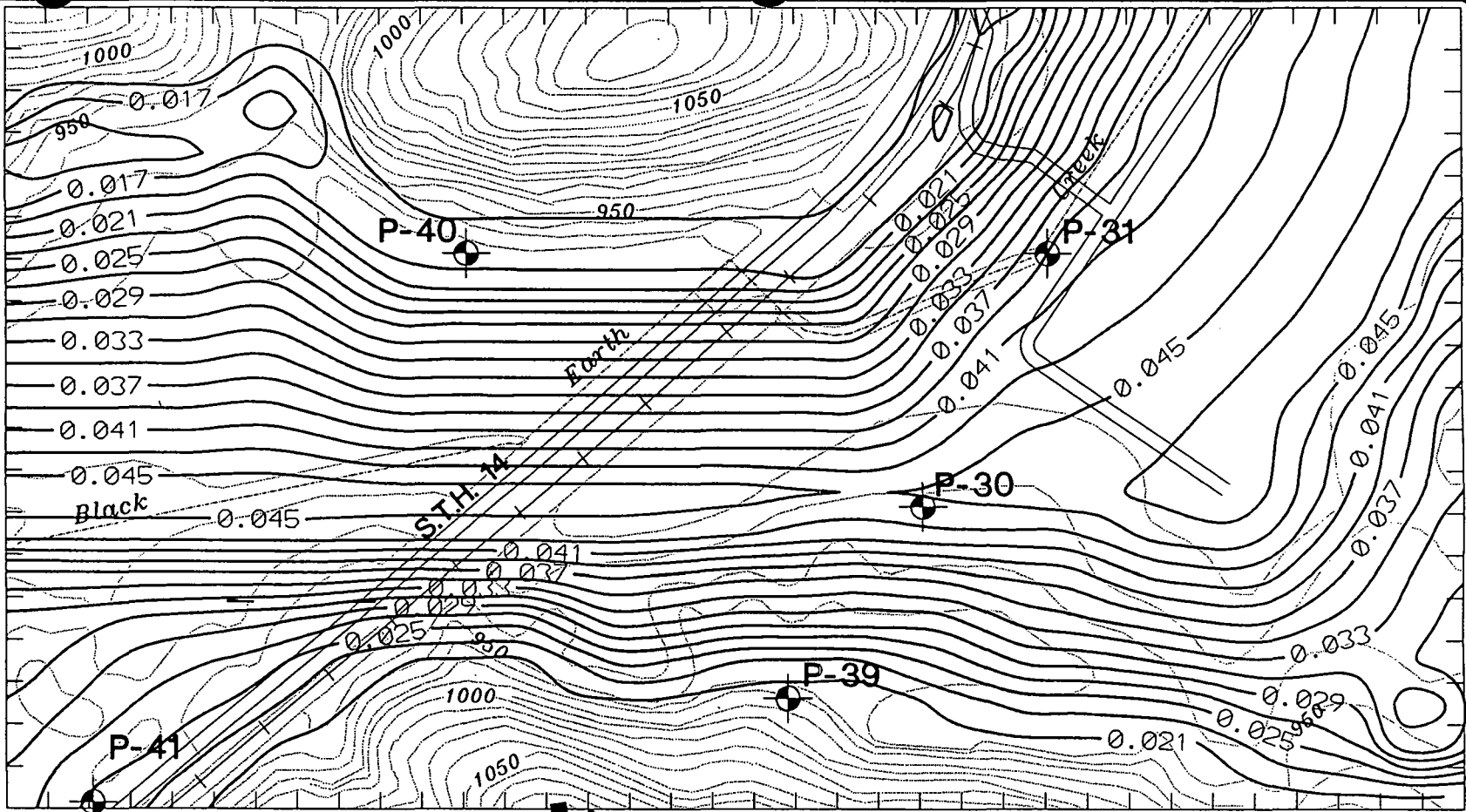
WISCONSIN DEPT. OF NATURAL RESOURCES
REFUSE HIDEAWAY LANDFILL

PCE PLUME WITHOUT
DEGRADATION AFTER 5 YEARS
(contour interval 2ppb)

| PROJECT: 148E13673 | DATE: 12/03/91 | DRAWING NO.: 1367-c17 | FIGURE: 4-20 |

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	30%	10%

12ppb - constant source
Base K's

EXPLANATION

P-30 ⬥ MONITOR WELL

—12.0— ISOCONCENTRATION CONTOUR

SCALE

0   500

FEET
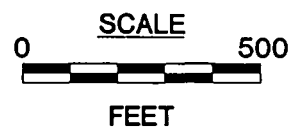
Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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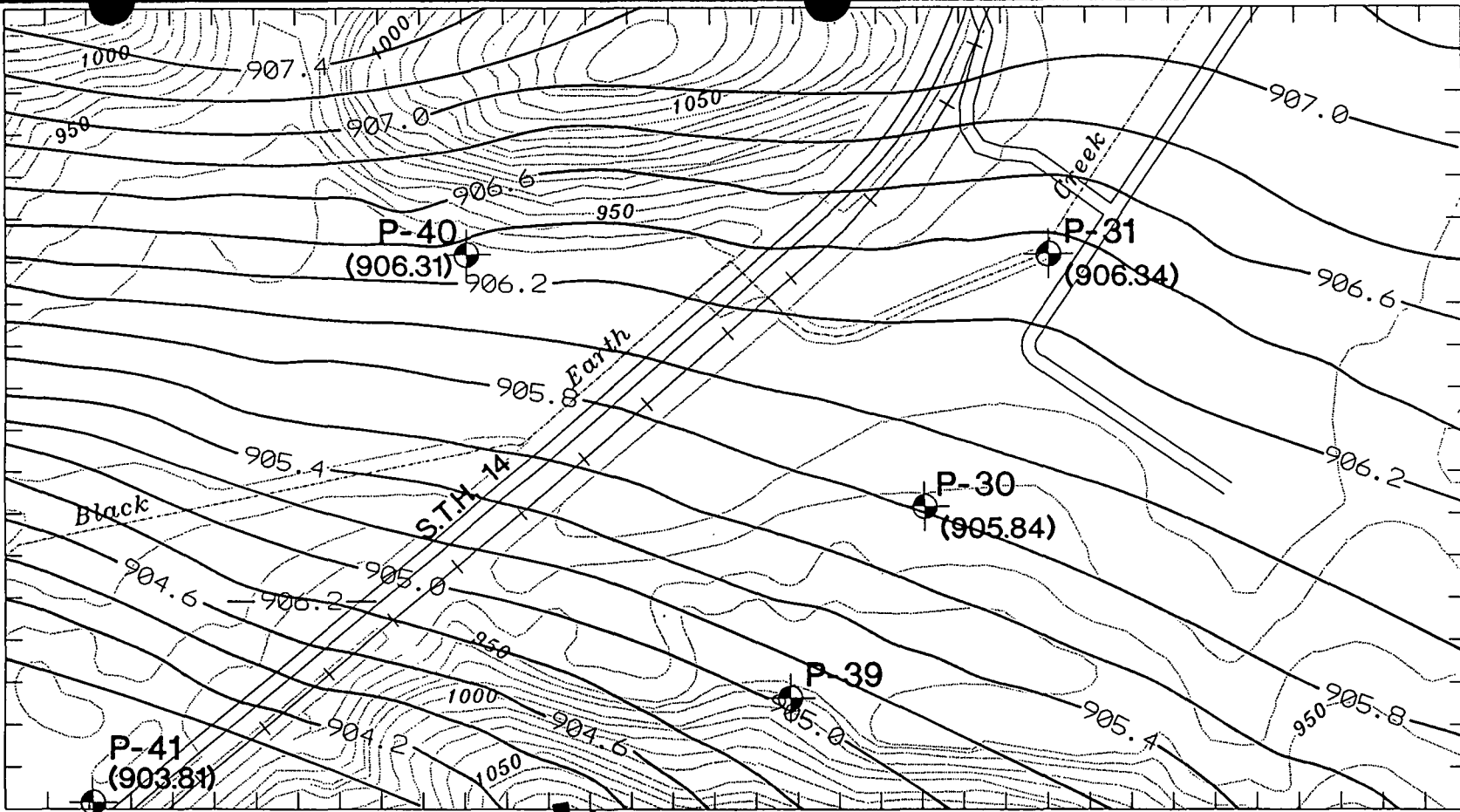WISCONSIN DEPT. OF NATURAL RESOURCES
REFUSE HIDEAWAY LANDFILL

**PCE PLUME WITH
DEGRADATION AFTER 5 YEARS**
(contour interval 2ppb)

PROJECT: 148E13673	DATE: 12/03/91	DRAWING NO.: 1367-c18	FIGURE: 4-21

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	30%	10%

12ppb - constant source
Base K's x10

EXPLANATION

P-30 ⊕ MONITOR WELL

—12.0— ISOCONCENTRATION CONTOUR

SCALE

0   500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

■ ◆ closest Deer Run homes
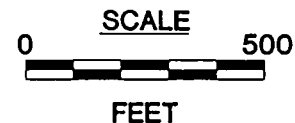
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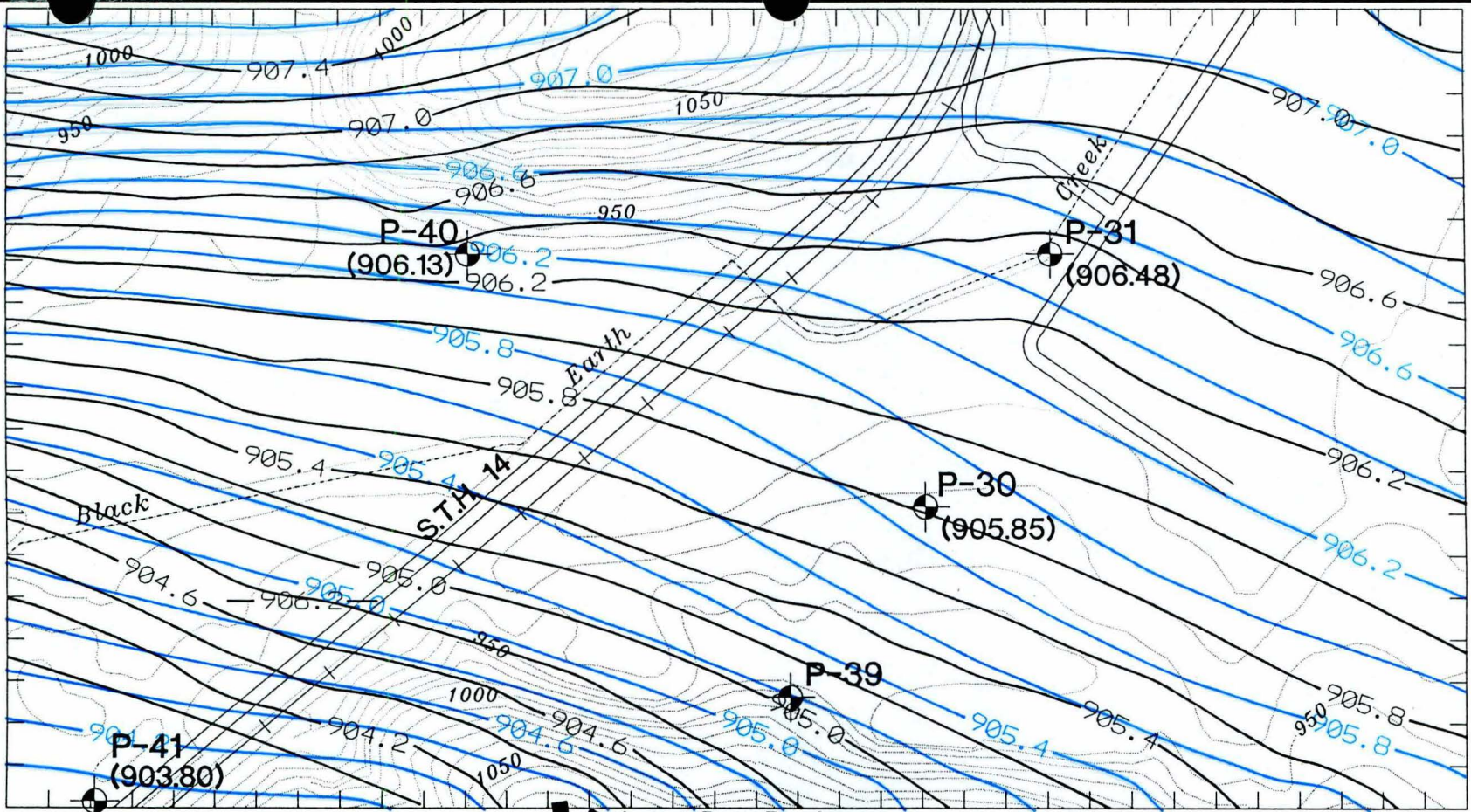WISCONSIN DEPT. OF NATURAL RESOURCES
REFUSE HIDEAWAY LANDFILL

PCE PLUME WITH
DEGRADATION AFTER 5 YEARS
(contour interval 2ppb)

PROJECT: 148E13673   DATE: 12/03/91   DRAWING NO.: 1367-c20   FIGURE: 4-22

PCE PLUME WITHOUT DEGRADATION AFTER 5 YEARS (contour interval 2ppb)

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	30%	10%

12ppb - constant source
Base K's

EXPLANATION

P-30-◆- MONITOR WELL

—12.0—— ISOCONCENTRATION CONTOUR

SCALE

0 _____ 500

FEET
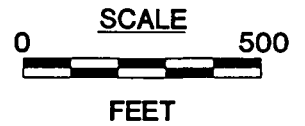
Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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PCE PLUME WITHOUT
DEGRADATION AFTER 5 YEARS
(contour interval 2ppb)

PROJECT: 148E13673   DATE: 12/03/91   DRAWING NO.: 1367-c19   FIGURE: 4-23

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	30%	10%

12ppb - constant source
Base K's x10

EXPLANATION

P-30-⬥ MONITOR WELL

—40.0—— ISOCONCENTRATION CONTOUR

◆ closest Deer Run homes

SCALE

0 ▮▮▮▮▮ 500

FEET
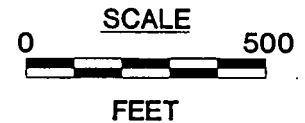
Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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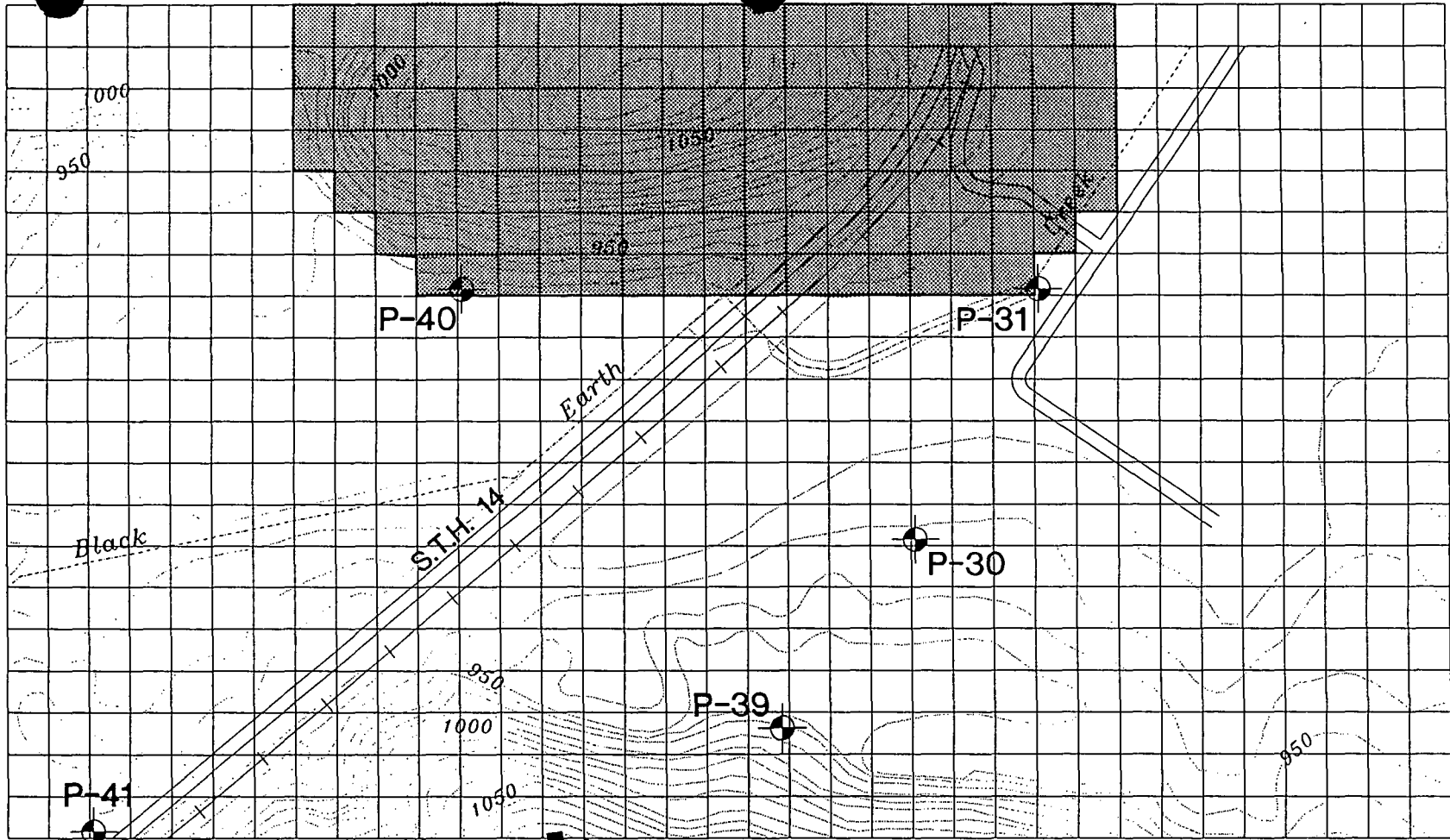REFUSE HIDEAWAY LANDFILL

**PCE PLUME WITH
DEGRADATION AFTER 5 YEARS**
(contour interval 2ppb)

PROJECT: 148E13673   DATE: 12/03/91   DRAWING NO.: 1367-c21   FIGURE: 4-24
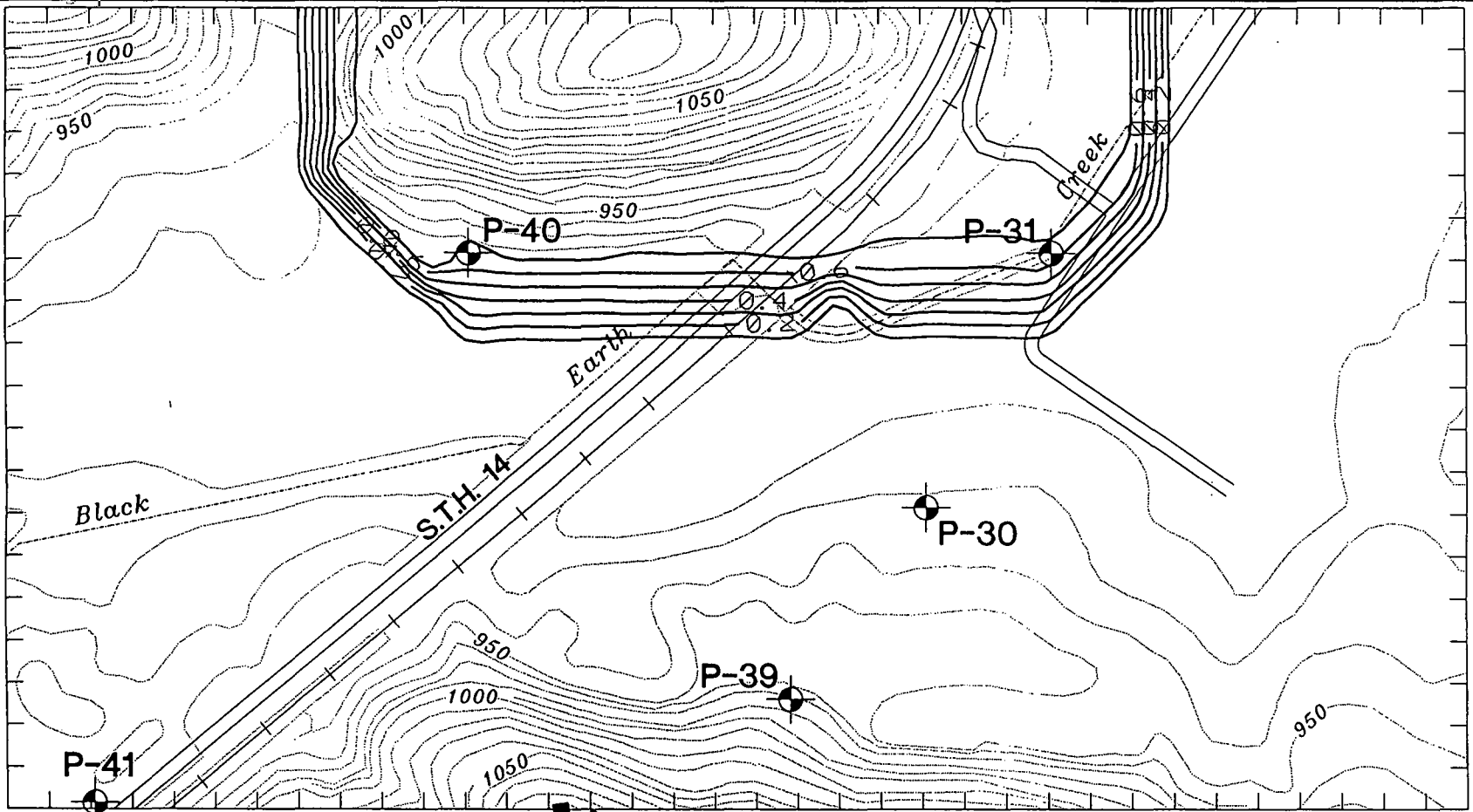
MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb – variable source
Base K's

EXPLANATION

P-30 ⌀ MONITOR WELL

— 0.4 — ISOCONCENTRATION CONTOUR
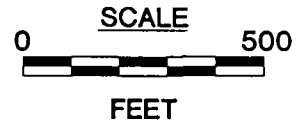
SCALE

0 ▬▬▬▬ 500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

■ ◆ closest Deer Run homes

P-40   P-31   P-30   P-39   P-41

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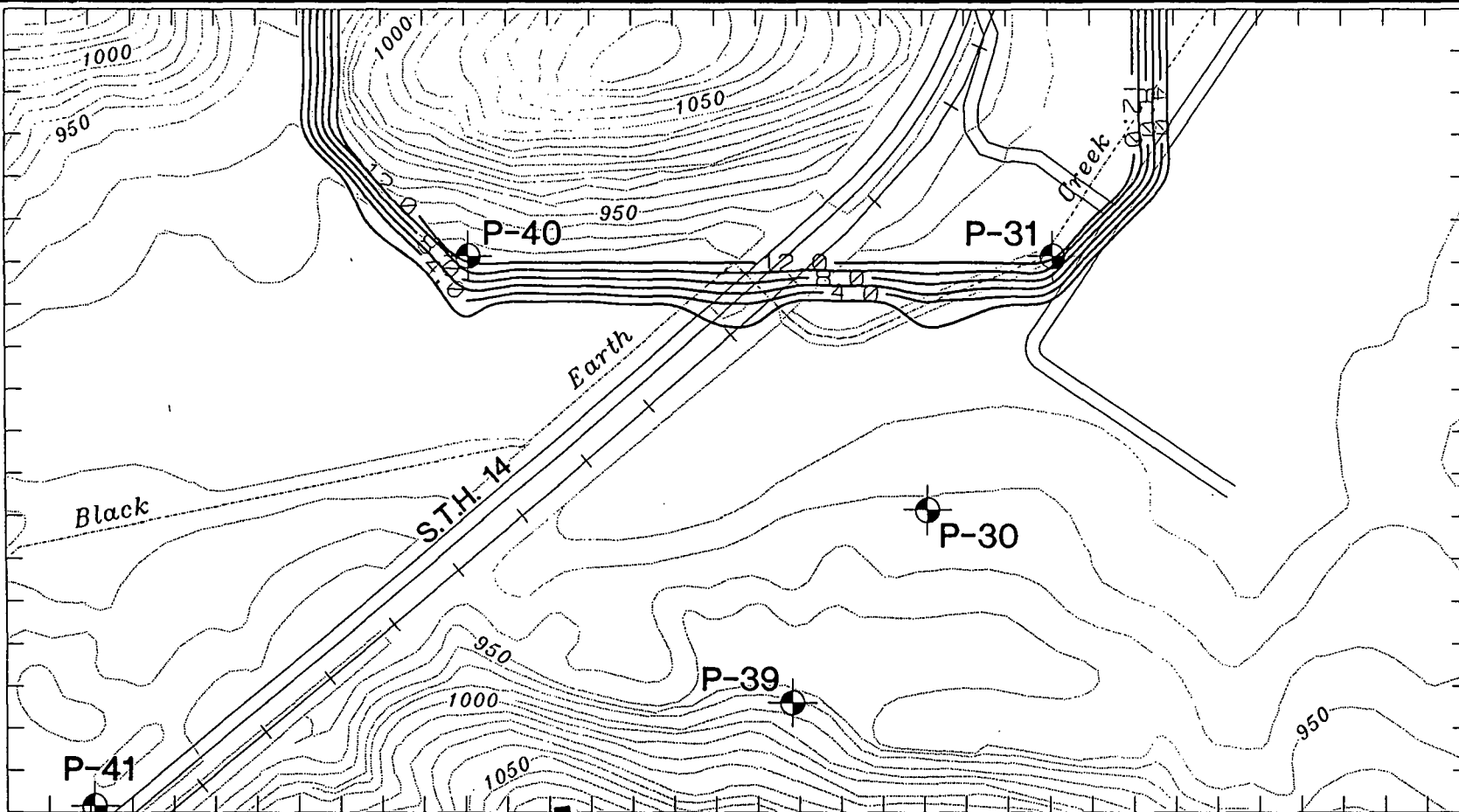WISCONSIN DEPT. OF NATURAL RESOURCES
REFUSE HIDEAWAY LANDFILL

PCE PLUME WITH
DEGRADATION AFTER 1.8 YEARS
(contour interval .2ppb)

PROJECT: 148E13673   DATE: 12/03/91   DRAWING NO.: 1367-c26d   FIGURE: 4-25
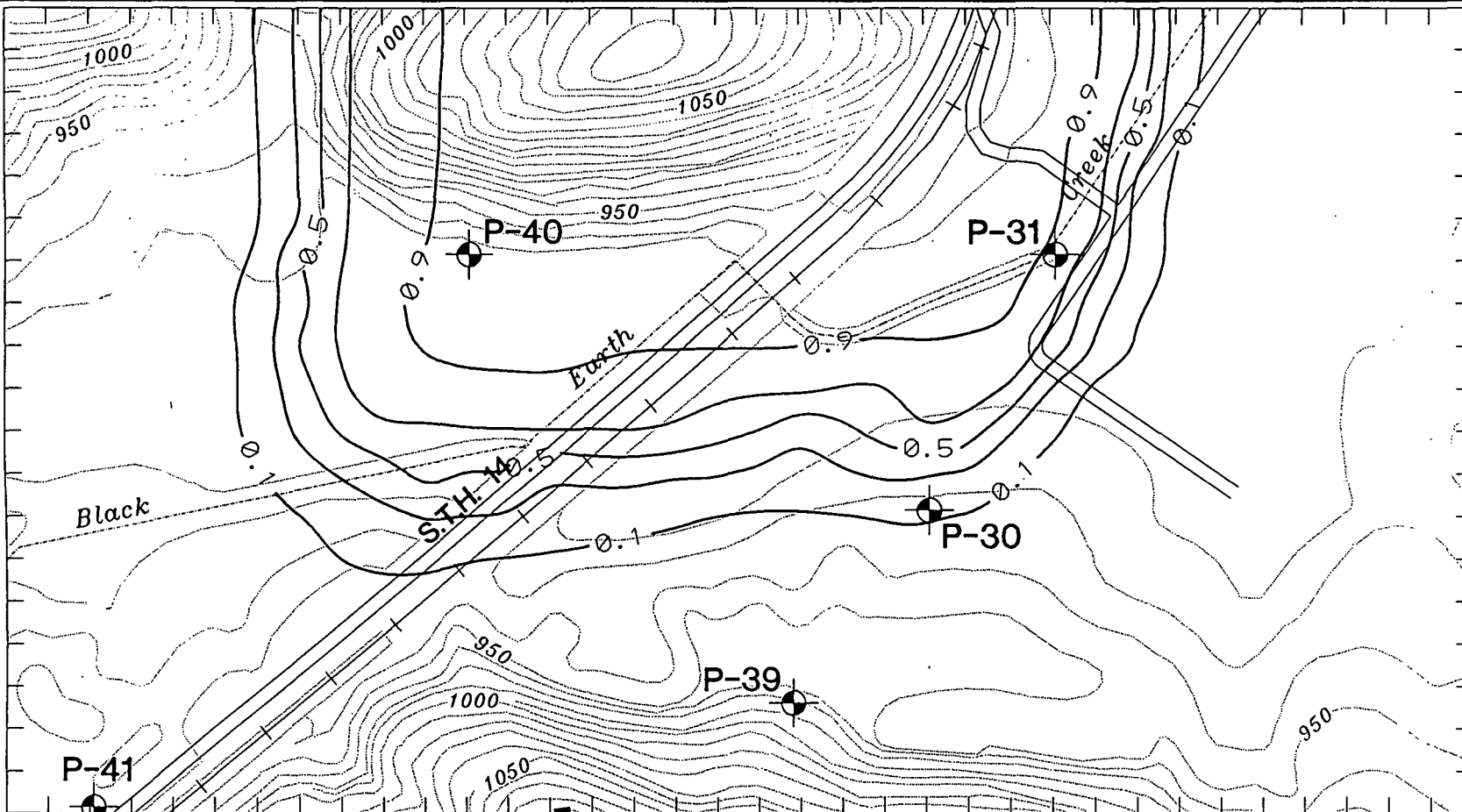
MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb - variable source
Base K's x10

EXPLANATION

P-30 ⬥ MONITOR WELL

— 0.5 — ISOCONCENTRATION CONTOUR
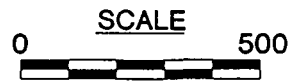
closest Deer Run homes

SCALE

0   500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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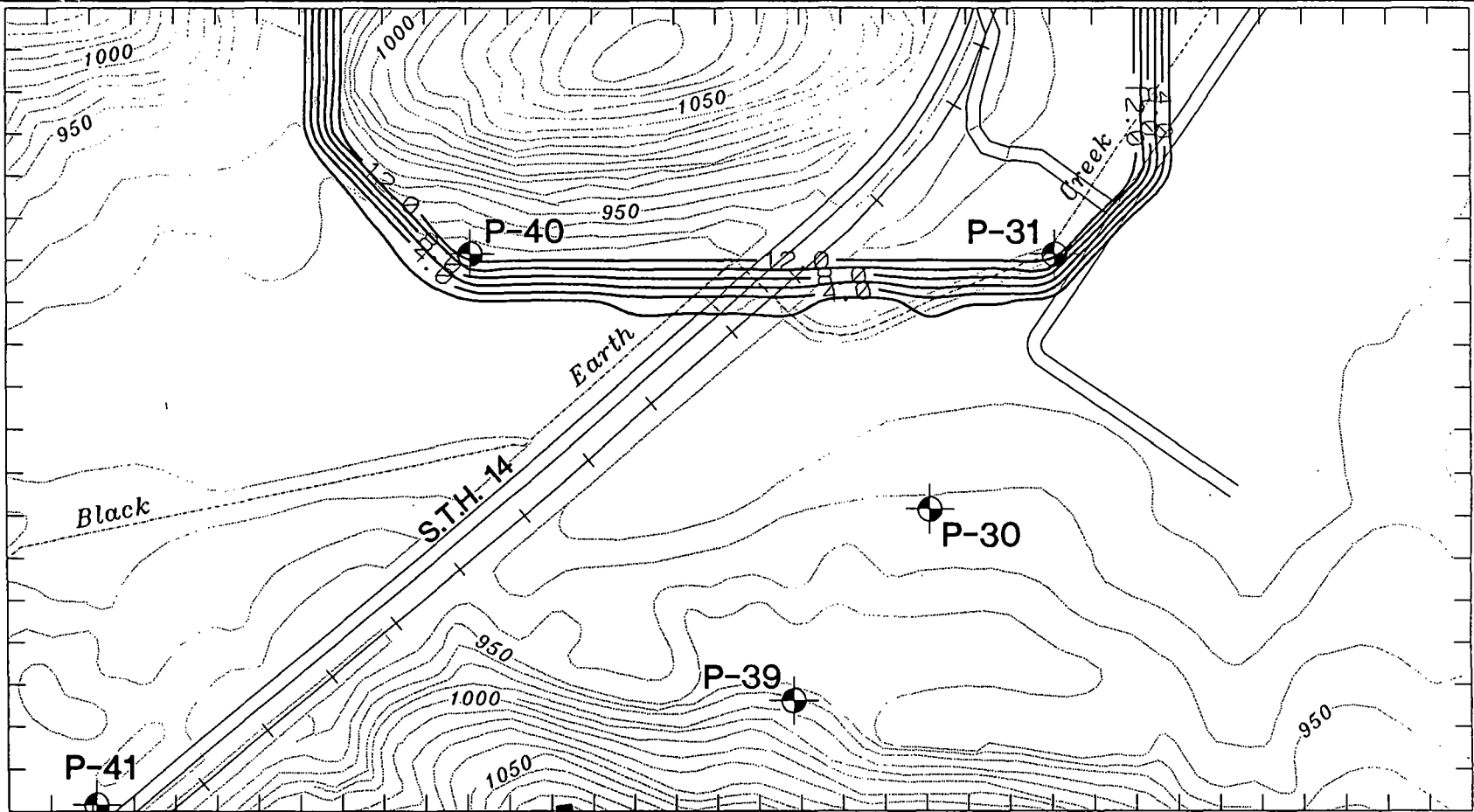WISCONSIN DEPT. OF NATURAL RESOURCES
REFUSE HIDEAWAY LANDFILL

PCE PLUME WITH
DEGRADATION AFTER 2.2 YEARS
(contour interval .2ppb)

PROJECT: 148E13673	DATE: 12/03/91	DRAWING NO.: 1367-c29	FIGURE: 4-26

P-40

P-31

P-30

P-39

P-41

● ◆ closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb – variable source
Base K's

EXPLANATION

P-30 ◆ MONITOR WELL

—— 4.0 —— ISOCONCENTRATION CONTOUR

SCALE

0   500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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WISCONSIN DEPT. OF NATURAL RESOURCES
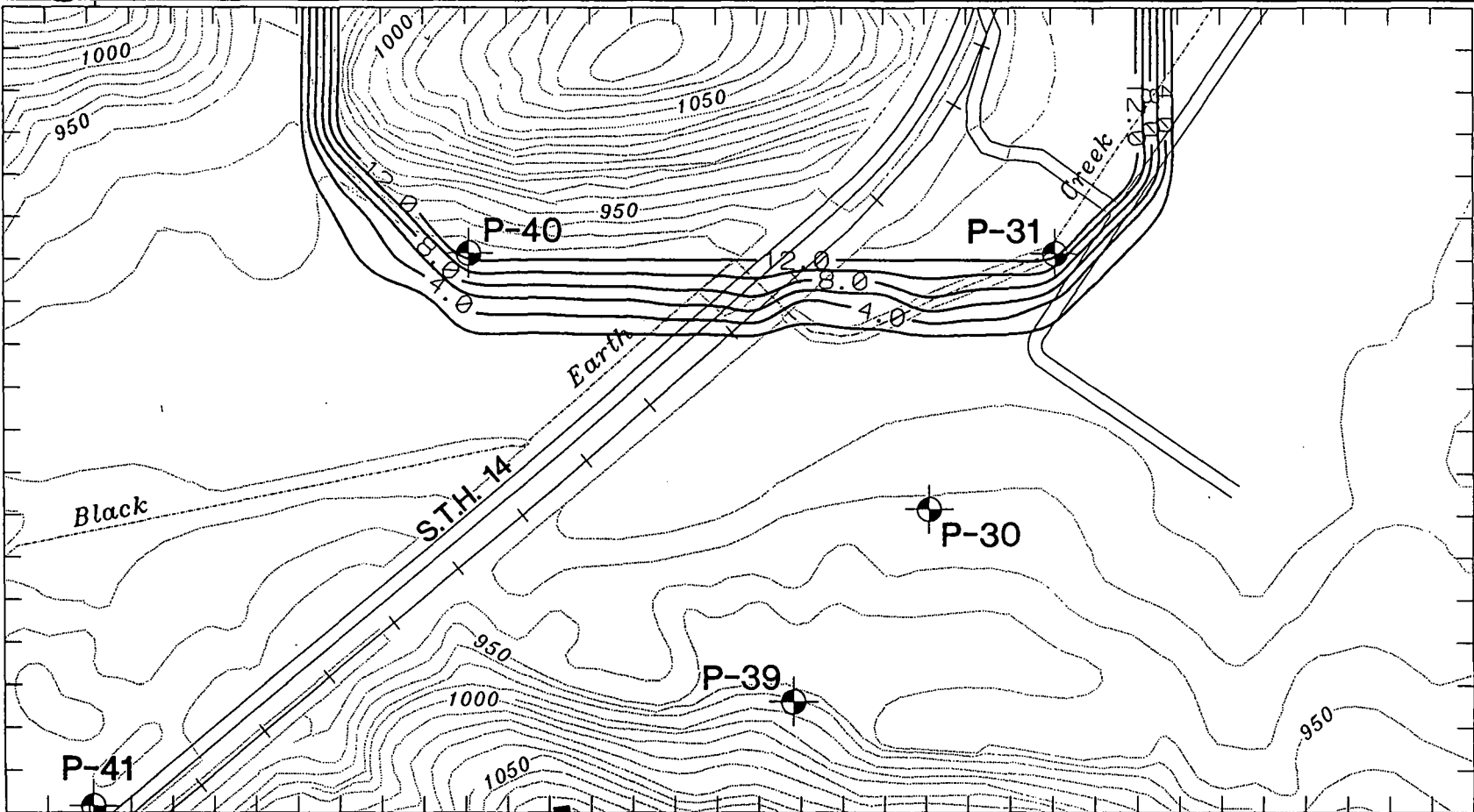REFUSE HIDEAWAY LANDFILL

PCE PLUME WITHOUT
DEGRADATION AFTER 22 YEARS
(contour interval 2ppb)
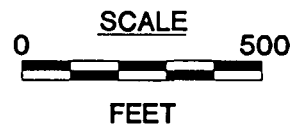
PROJECT: 148E13673	DATE: 12/03/91	DRAWING NO.: 1367-c28a	FIGURE: 4-27
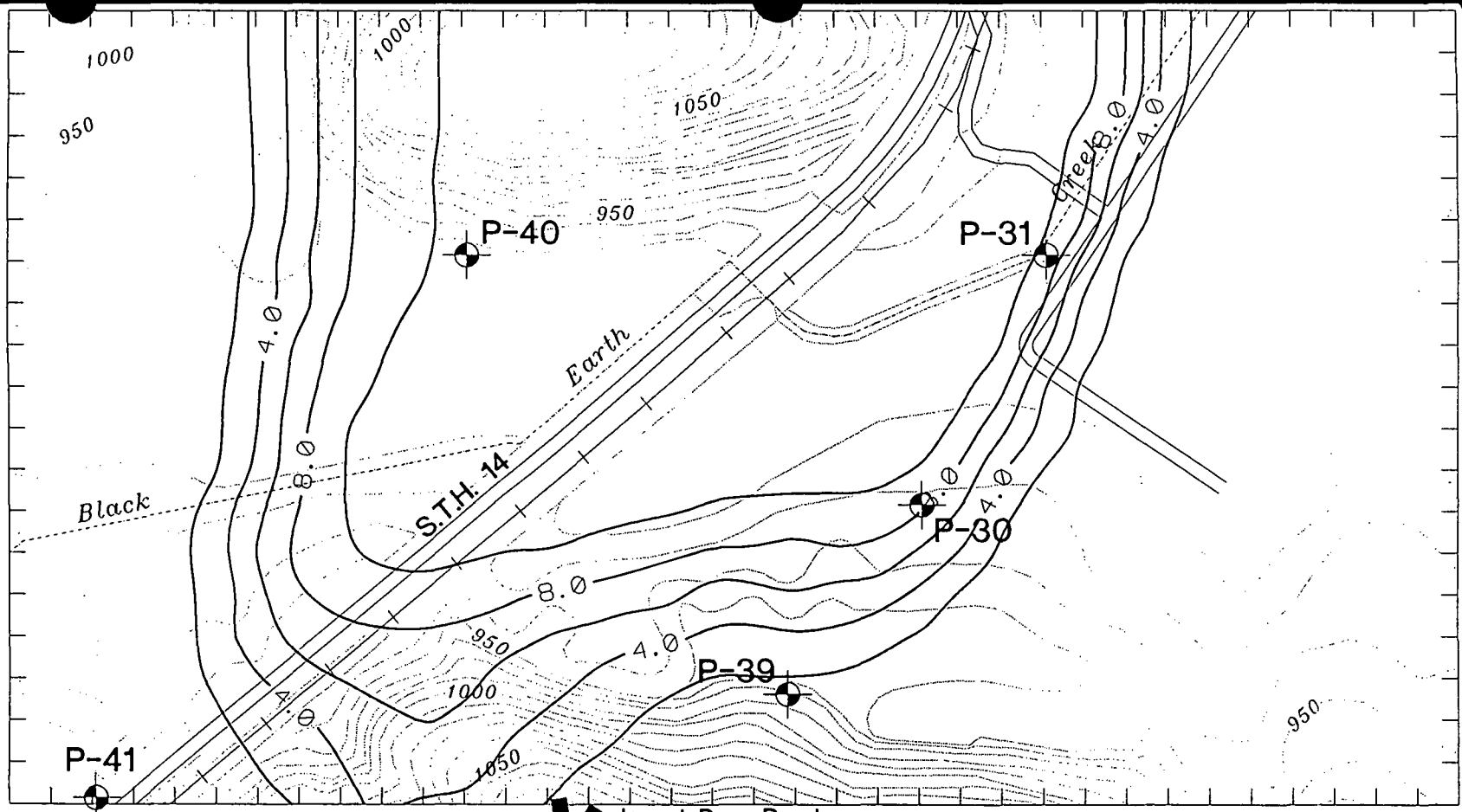
P-40

P-31

P-30

P-39

P-41

Black

Earth

S.T.H. 14

Creek

1000
950
1050
950
1000
950
1050
1000

4.0
8.0
8.0
8.0
4.0
4.0
8.0
4.0

■◆ closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb - variable source
Base K's

EXPLANATION

P-30 ◆ MONITOR WELL

—— 4.0 —— ISOCONCENTRATION CONTOUR

SCALE

0 ————————— 500

FEET
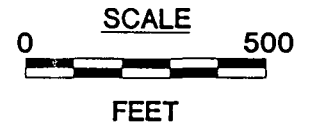
Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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PCE PLUME WITHOUT
DEGRADATION AFTER 45 YEARS
(contour interval 2ppb)

| PROJECT: 148E13673	DATE: 12/03/91	DRAWING NO.: 1367-c28b	FIGURE: 4-28
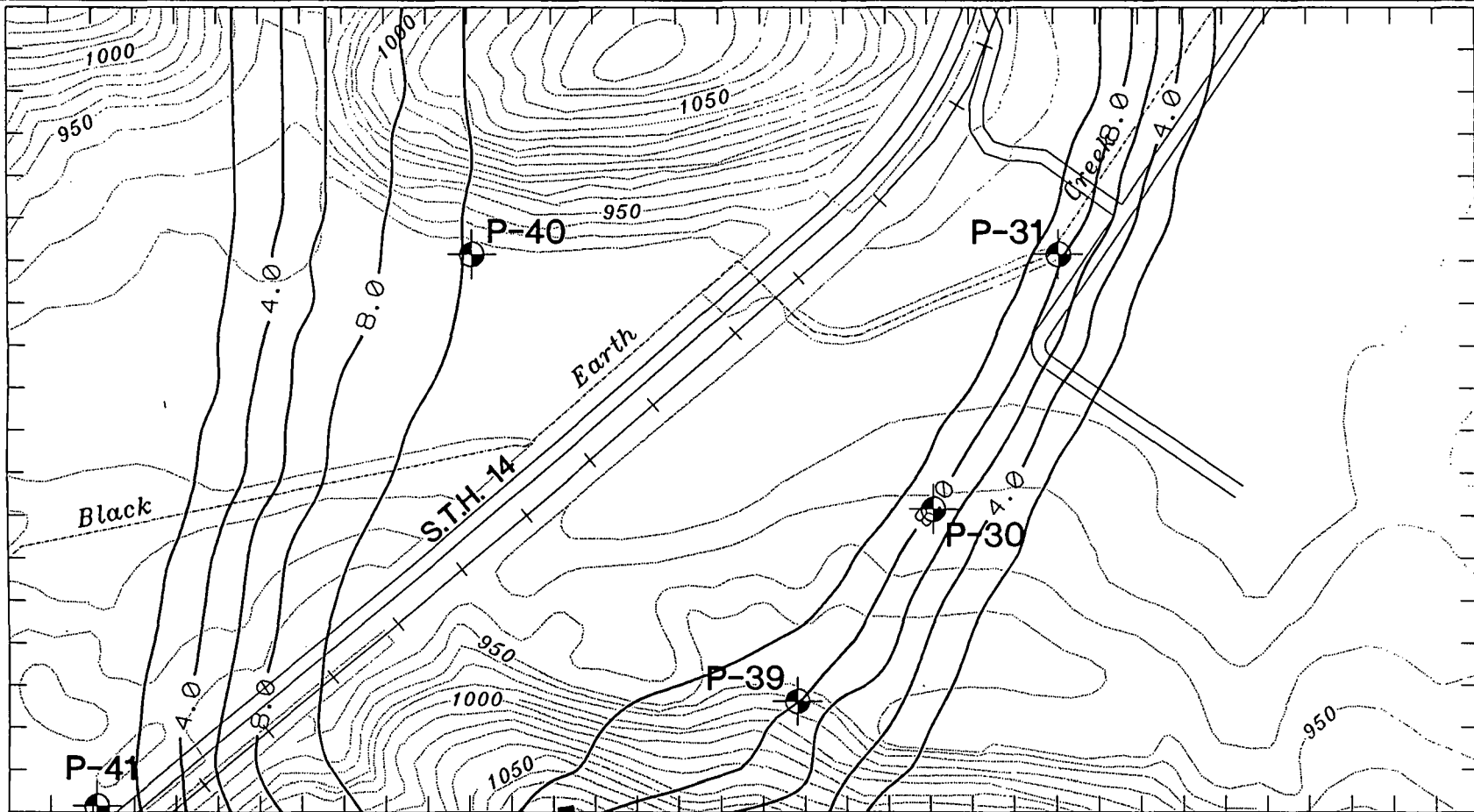
P-40

P-31

Creek

Earth

Black

S.T.H. 14

P-30

P-39

P-41

closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb - variable source
Base K's

EXPLANATION

P-30 ⬥ MONITOR WELL

— 4.0 — ISOCONCENTRATION CONTOUR

SCALE

0 ——————— 500

FEET
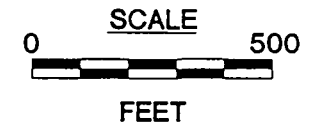
Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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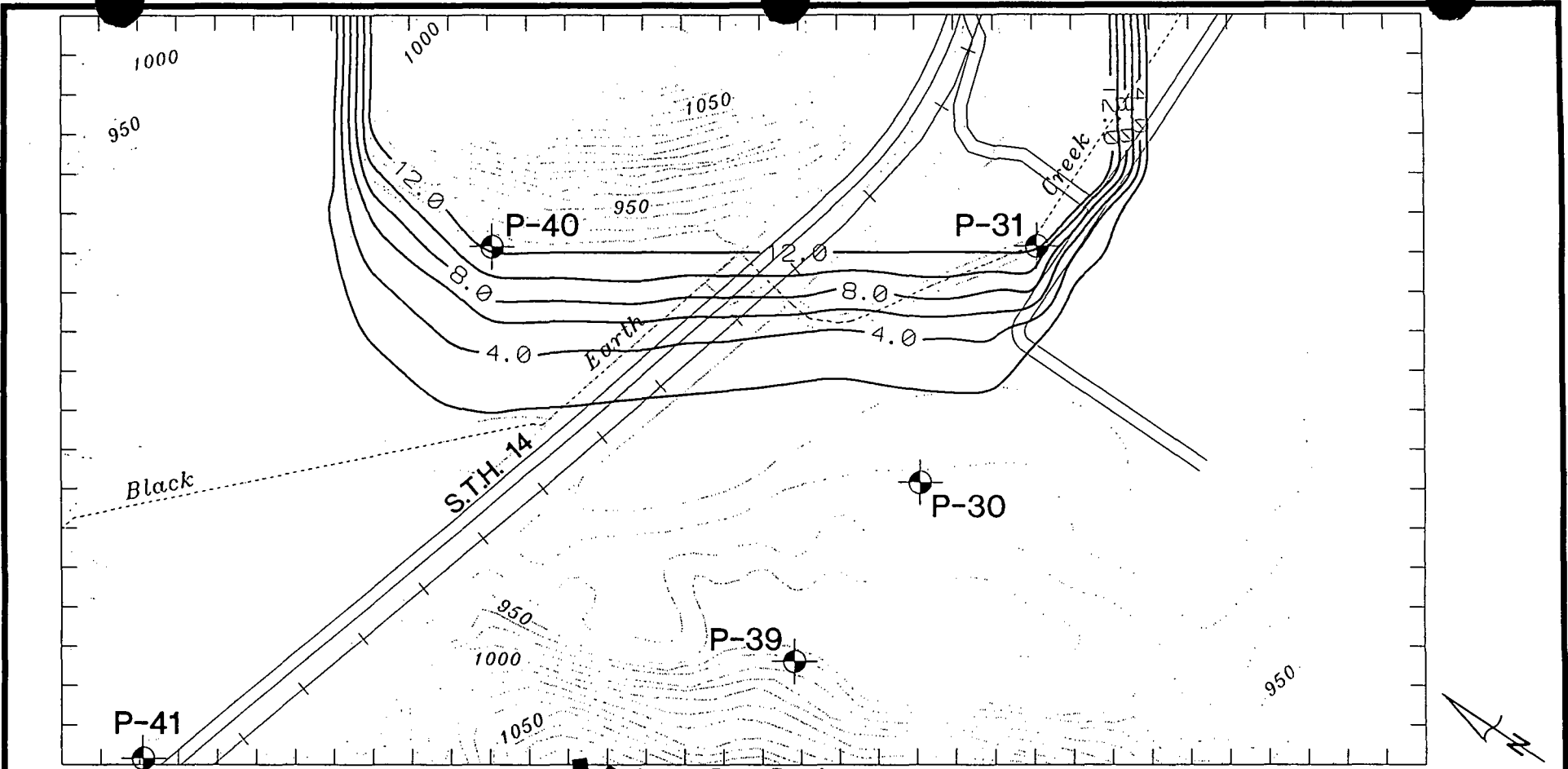WISCONSIN DEPT. OF NATURAL RESOURCES
REFUSE HIDEAWAY LANDFILL

PCE PLUME WITHOUT
DEGRADATION AFTER 75 YEARS
(contour interval 2ppb)

PROJECT: 148E13673	DATE: 12/03/91	DRAWING NO.: 1367-c28c	FIGURE: 4-29

P-40

P-31

P-30

P-39

P-41

■◆ closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb – variable source
Base K's x10

EXPLANATION

P-30-◆- MONITOR WELL

— 4.0 — ISOCONCENTRATION CONTOUR

SCALE

0 _____ 500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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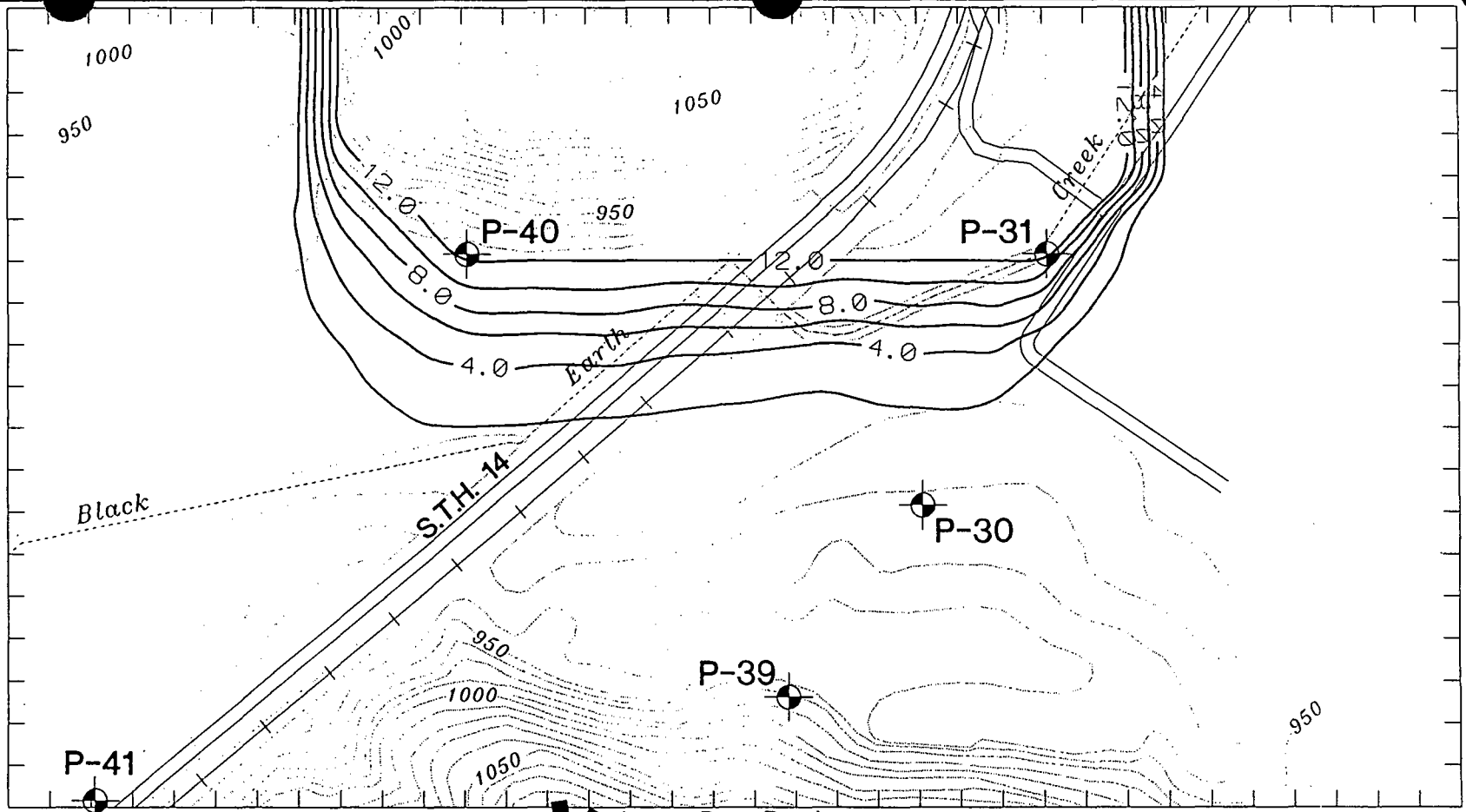WISCONSIN DEPT. OF NATURAL RESOURCES
REFUSE HIDEAWAY LANDFILL

PCE PLUME WITHOUT DEGRADATION AFTER 2.2 YEARS
(contour interval 2ppb)
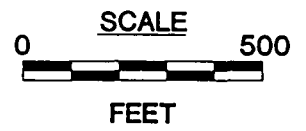
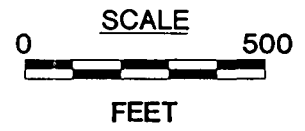| PROJECT: 148E13673 | DATE: 12/03/91 | DRAWING NO.: 1367-c30b | FIGURE: 4-30 |

PCE PLUME WITHOUT DEGRADATION AFTER 4.2 YEARS (contour interval 2ppb)

Map labels:
- P-40
- P-31
- P-30
- P-39
- P-41
- S.T.H. 14
- Earth
- Black
- Creek
- closest Deer Run homes
- 1000, 950, 1050 (topographic contours)
- 4.0, 8.0 (isoconcentration contours)

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb - variable source
Base K's x10

EXPLANATION

P-30 ⬥ MONITOR WELL

— 4.0 — ISOCONCENTRATION CONTOUR

SCALE

0 ————— 500

FEET
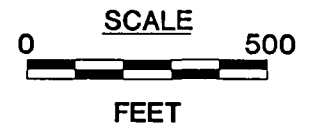
Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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PCE PLUME WITHOUT
DEGRADATION AFTER 4.2 YEARS
(contour interval 2ppb)

PROJECT: 148E13673   DATE: 12/03/91   DRAWING NO.: 1367-c30c   FIGURE: 4-31
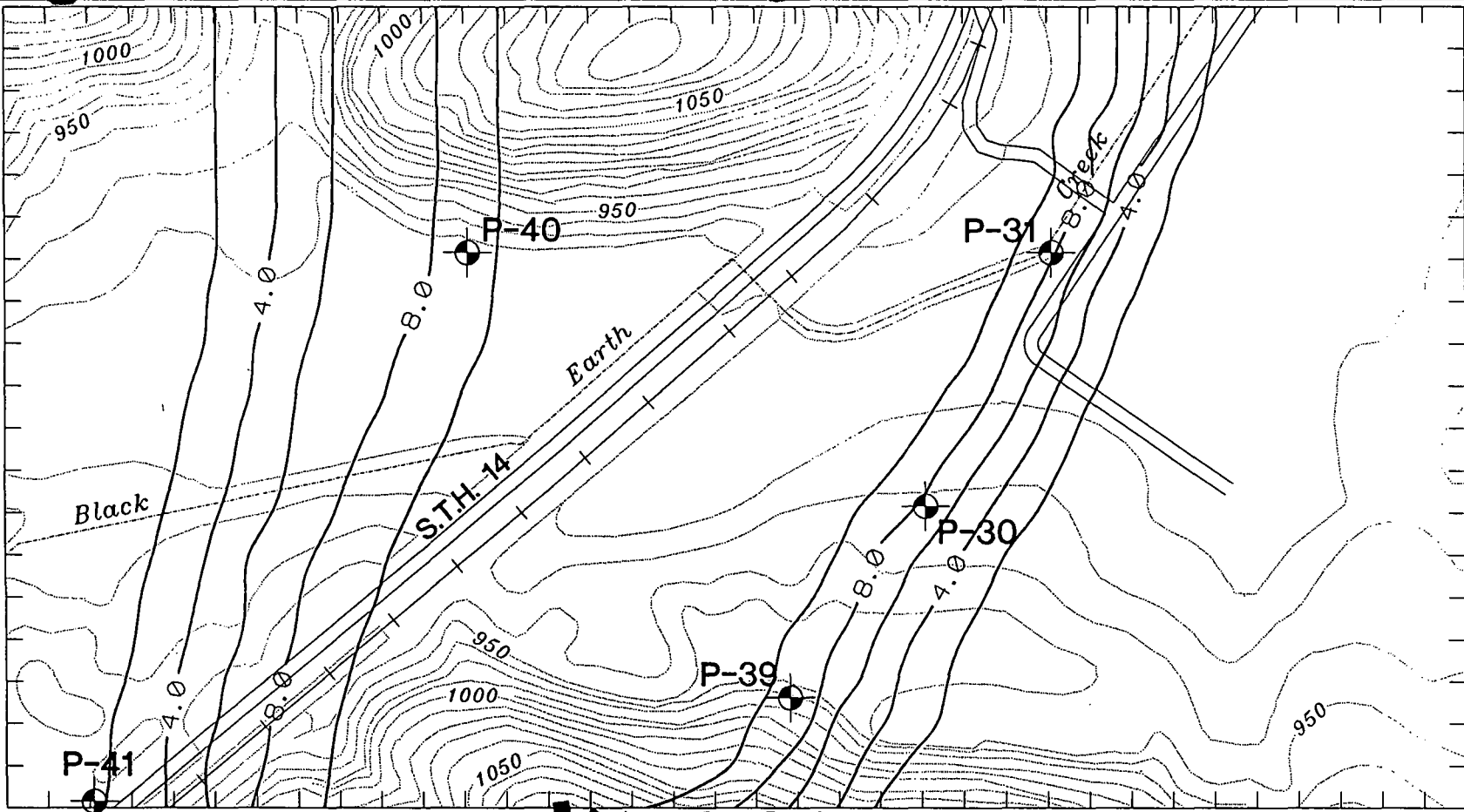
MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb – variable source
Base K's x10

EXPLANATION

P-30 ⊕ MONITOR WELL

— 4.0 — ISOCONCENTRATION CONTOUR

SCALE
0   500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

◼◆ closest Deer Run homes
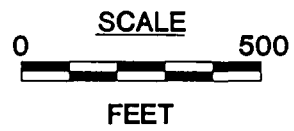
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PCE PLUME WITHOUT
DEGRADATION AFTER 10 YEARS
(contour interval 2ppb)

PROJECT: 148E13673	DATE: 12/03/91	DRAWING NO.: 1367-c30a	FIGURE: 4-32

closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb - constant source
Base K's

EXPLANATION

P-30-⊕ MONITOR WELL

—12.0—— ISOCONCENTRATION CONTOUR

SCALE

0   500

FEET
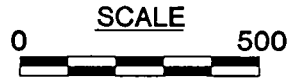
Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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WISCONSIN DEPT. OF NATURAL RESOURCES
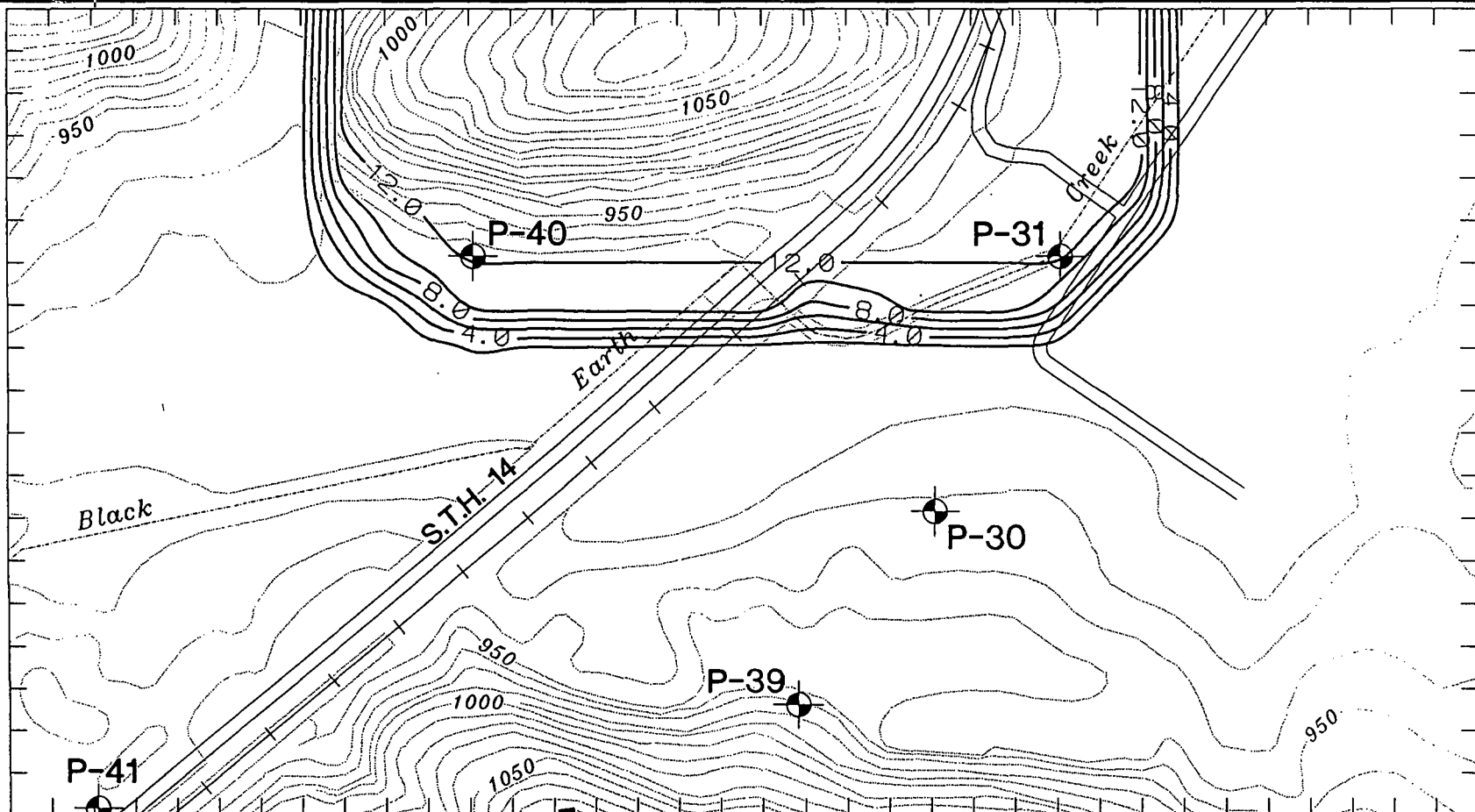REFUSE HIDEAWAY LANDFILL

**PCE PLUME WITHOUT
DEGRADATION AFTER 20 YEARS**
(contour interval 2ppb)

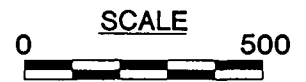| PROJECT: 148E13673 | DATE: 12/03/91 | DRAWING NO.: 1367-c3d | FIGURE: 4-33 |
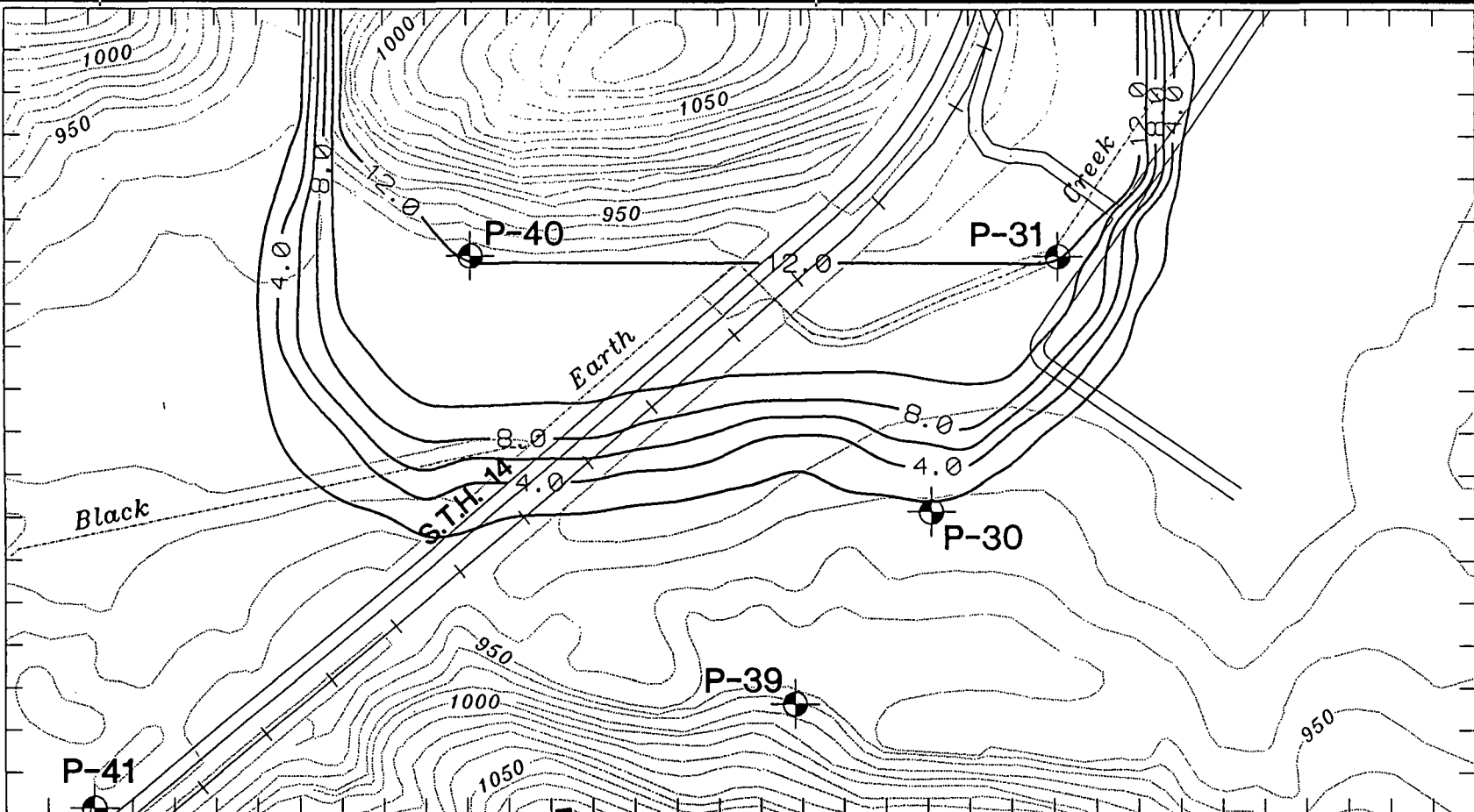
closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb - constant source
Base K's x10

EXPLANATION

P-30-⬦ MONITOR WELL

— 4.0 — ISOCONCENTRATION CONTOUR

SCALE

0 — 500

FEET
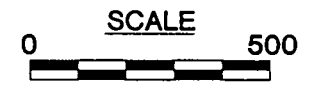
Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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WISCONSIN DEPT. OF NATURAL RESOURCES
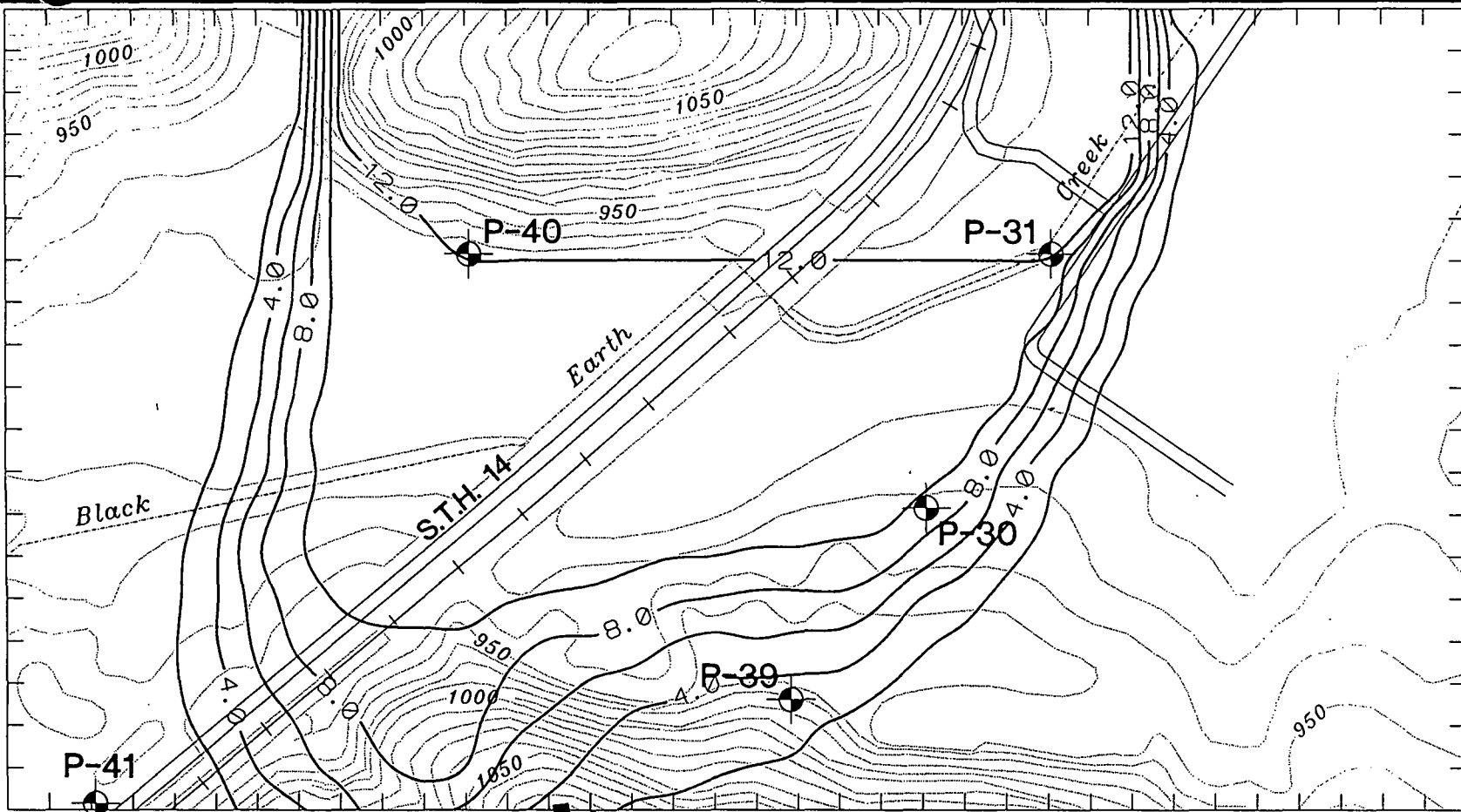REFUSE HIDEAWAY LANDFILL

PCE PLUME WITHOUT DEGRADATION AFTER 2.1 YEARS
(contour interval 2ppb)

PROJECT: 148E13673 | DATE: 12/03/91 | DRAWING NO.: 1367-c4a | FIGURE: 4-34

closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb - constant source
Base K's x10

EXPLANATION

P-30 ⊕ MONITOR WELL

— 4.0 — ISOCONCENTRATION CONTOUR

SCALE

0 — 500

FEET
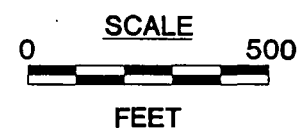
Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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REFUSE HIDEAWAY LANDFILL

PCE PLUME WITHOUT DEGRADATION AFTER 4.1 YEARS
(contour interval 2ppb)

PROJECT: 148E13673	DATE: 12/03/91	DRAWING NO.: 1367-c4c	FIGURE: 4-35

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb – constant source
Base K's

EXPLANATION

P-30-⦵ MONITOR WELL

—12.0—— ISOCONCENTRATION CONTOUR

SCALE

0 _____ 500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

● closest Deer Run homes
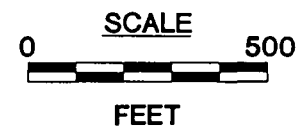
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WISCONSIN DEPT. OF NATURAL RESOURCES
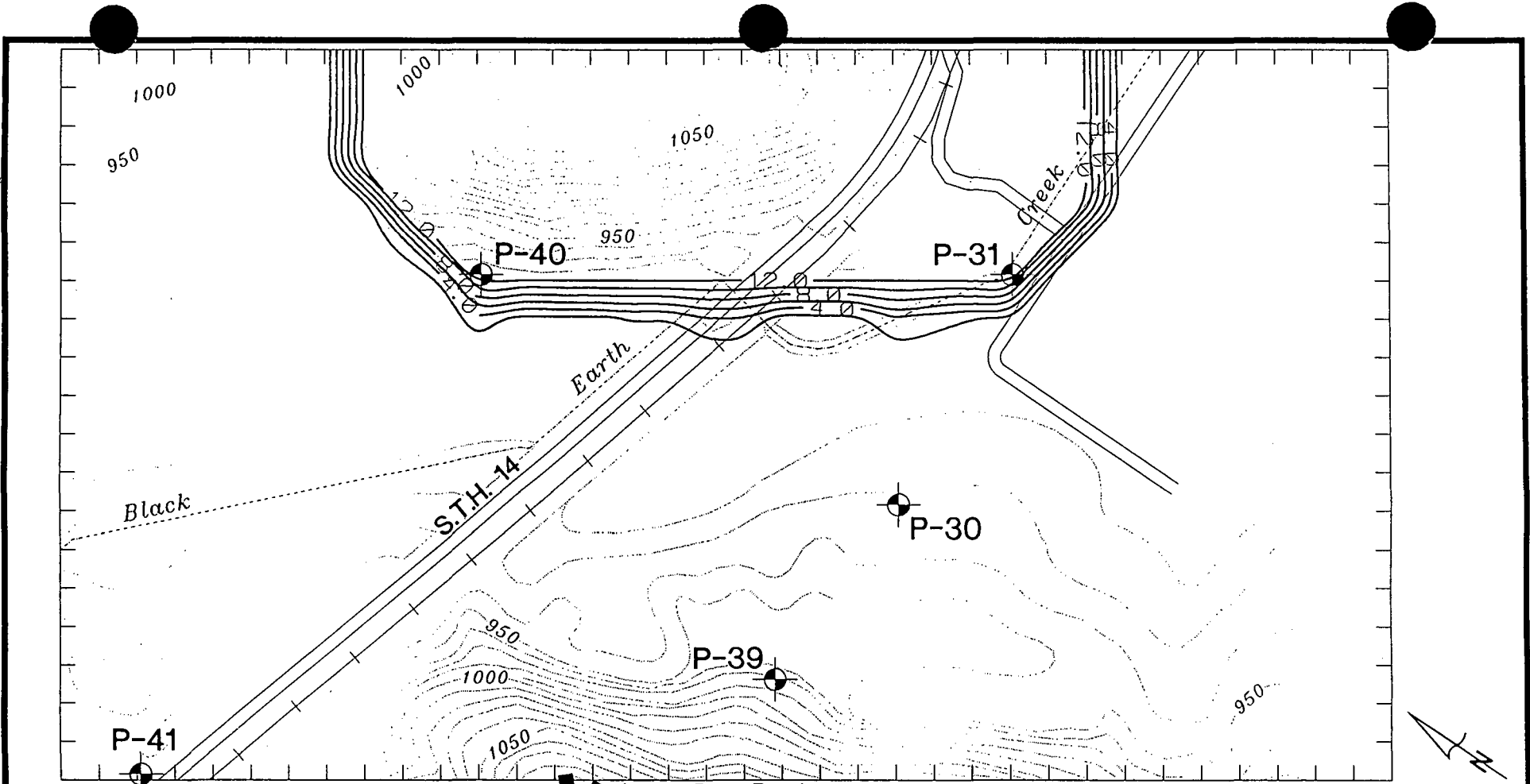REFUSE HIDEAWAY LANDFILL

PCE PLUME WITHOUT
DEGRADATION AFTER 40 YEARS
(contour interval 2ppb)

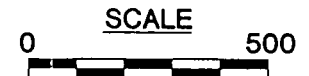| PROJECT: 148E13673 | DATE: 12/03/91 | DRAWING NO.: 1367-c3f | FIGURE: 4-36 |
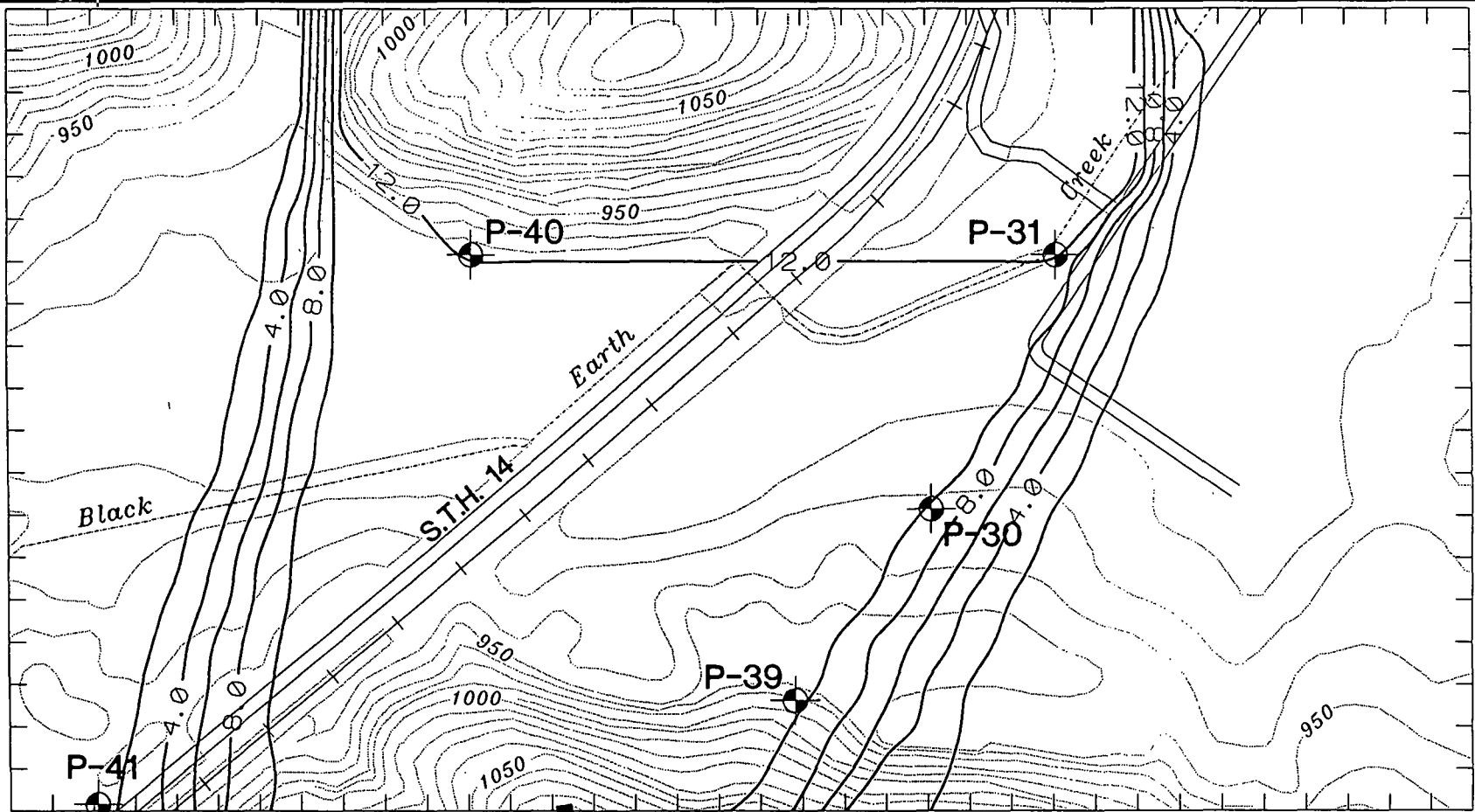
MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb – constant source
Base K's x10

EXPLANATION

P-30 ⬥ MONITOR WELL

— 4.0 — ISOCONCENTRATION CONTOUR

◆ closest Deer Run homes

SCALE
0 — 500
FEET
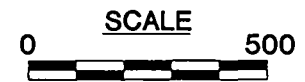
Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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WISCONSIN DEPT. OF NATURAL RESOURCES
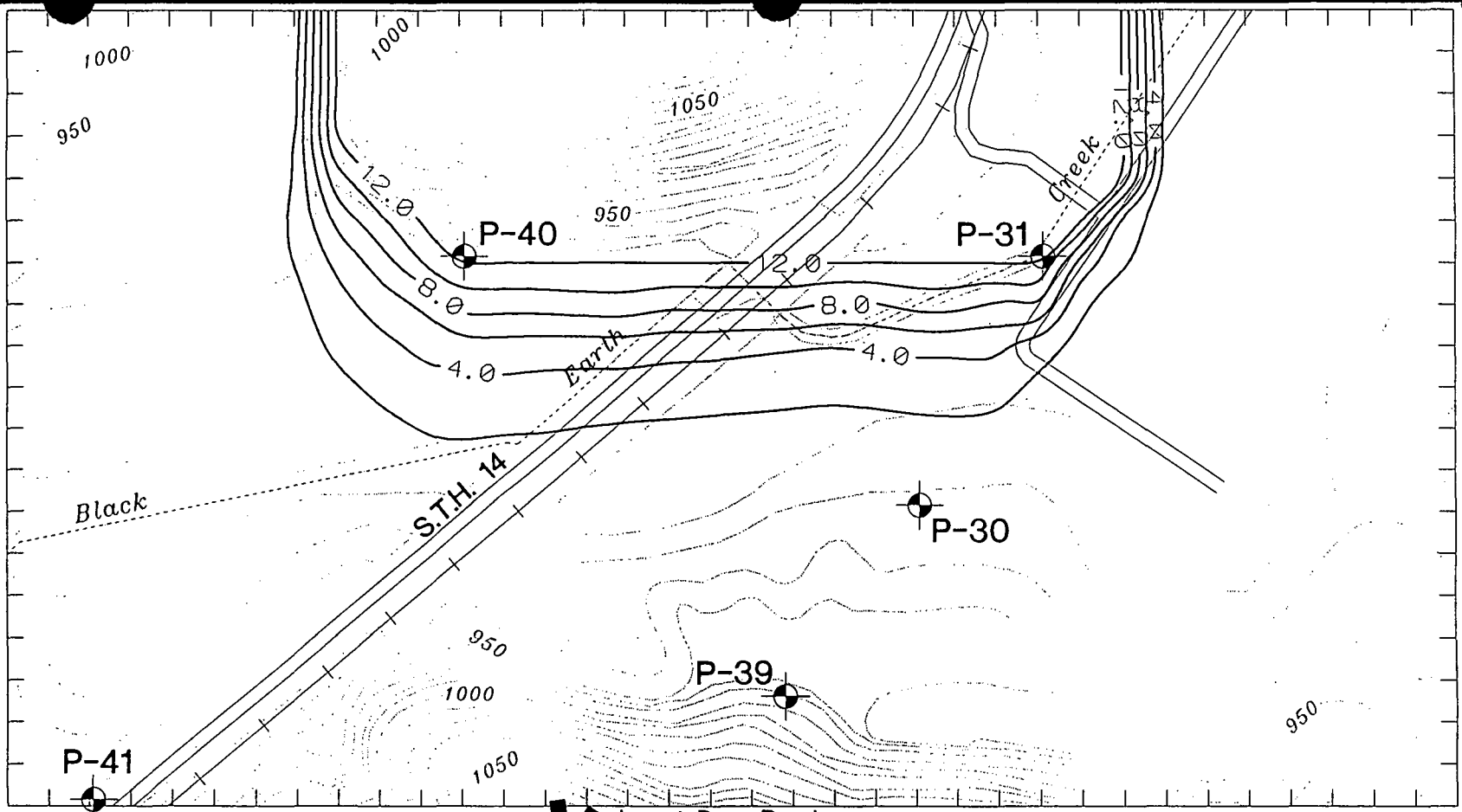REFUSE HIDEAWAY LANDFILL

PCE PLUME WITHOUT
DEGRADATION AFTER 9 YEARS
(contour interval 2ppb)

PROJECT: 148E13673   DATE: 12/03/91   DRAWING NO.: 1367-c4b   FIGURE: 4-37

Labels on map: 1000, 950, 1050, 950, P-40, P-31, Creek, Earth, Black, S.T.H.-14, 12.0, 4.0, 8.0, P-30, P-39, 950, 1000, 1050, P-41, 950

■ ◆ closest Deer Run homes

MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb - constant source
Base K's

EXPLANATION

P-30-◆ MONITOR WELL

—12.0—— ISOCONCENTRATION CONTOUR

SCALE

0 — 500

FEET

Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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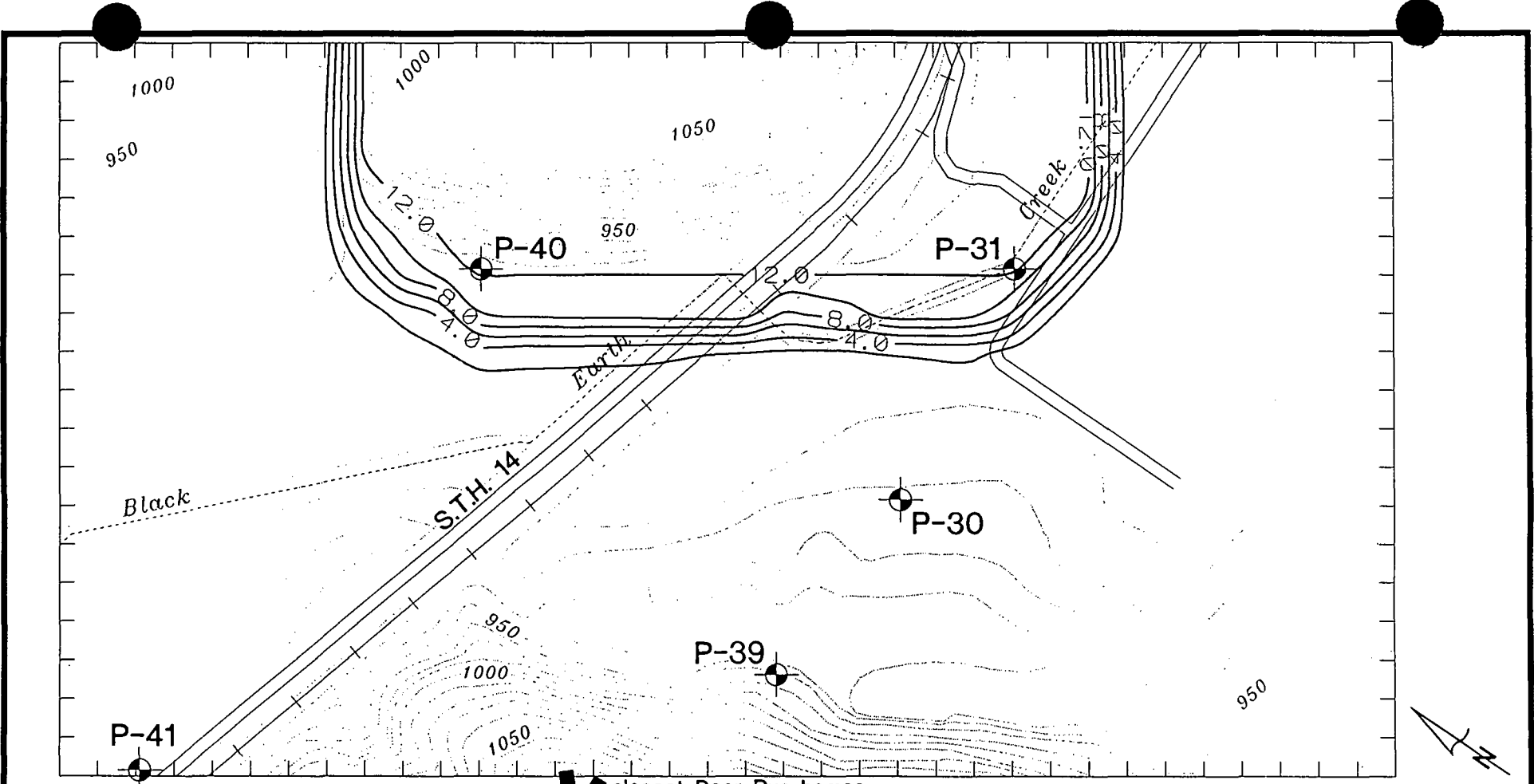WISCONSIN DEPT. OF NATURAL RESOURCES
REFUSE HIDEAWAY LANDFILL

PCE PLUME WITHOUT
DEGRADATION AFTER 100 YEARS
(contour interval 2ppb)
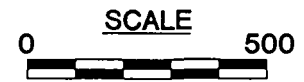
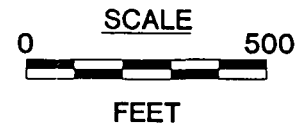PROJECT: 148E13673   DATE: 12/03/91   DRAWING NO.: 1367-c3a   FIGURE: 4-38
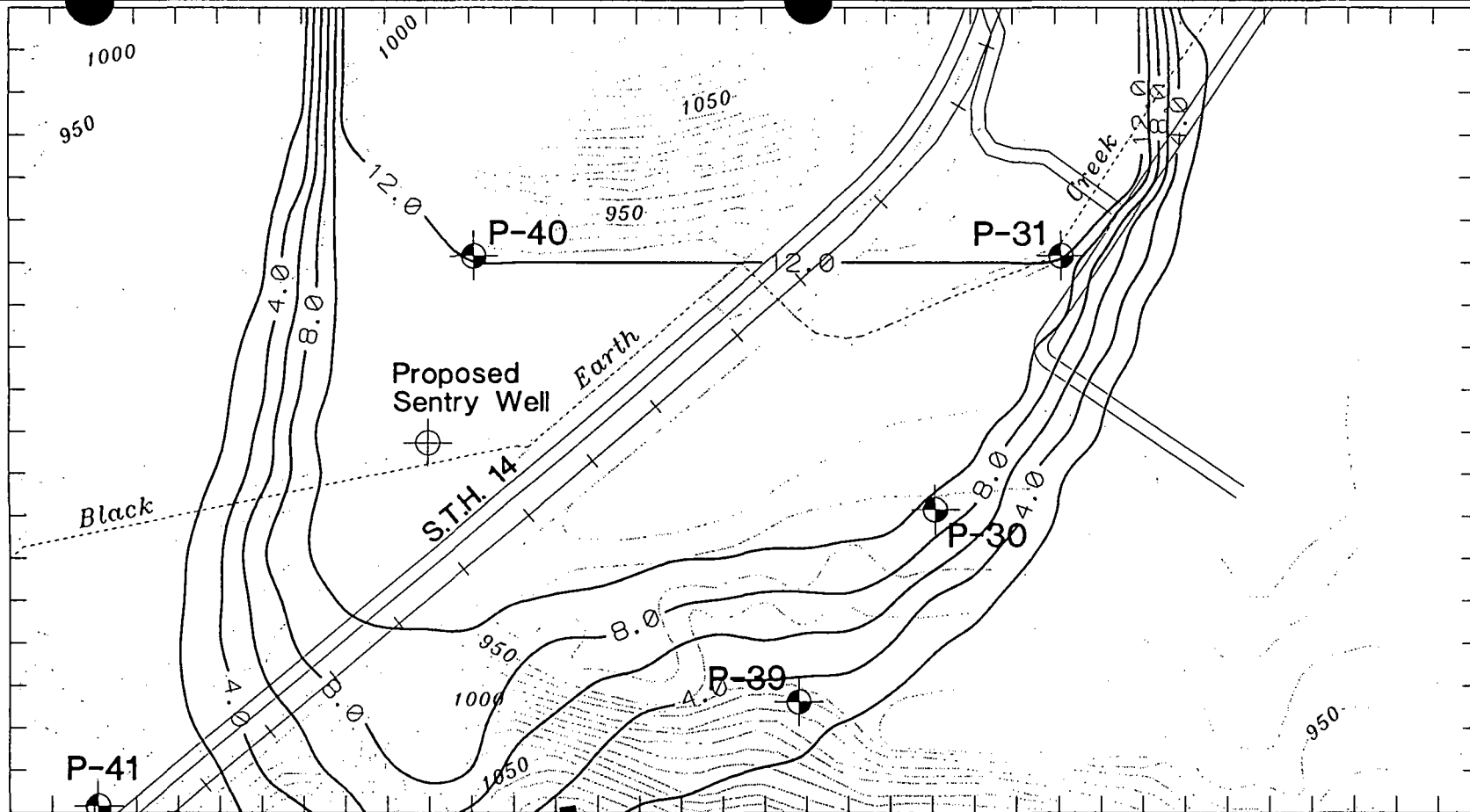
MODEL CONDITIONS

	s/g	bedrock
DISPERSIVITY	30ft.	10ft.
EFFECTIVE POROSITY	25%	5%

12ppb - constant source
Base K's x10

EXPLANATION

P-30 ⌖ MONITOR WELL

— 4.0 — ISOCONCENTRATION CONTOUR

SCALE

0 ————————— 500

FEET
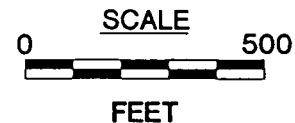
Topographic Contour Interval 10ft.
Datum is Mean Sea Level

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WISCONSIN DEPT. OF NATURAL RESOURCES
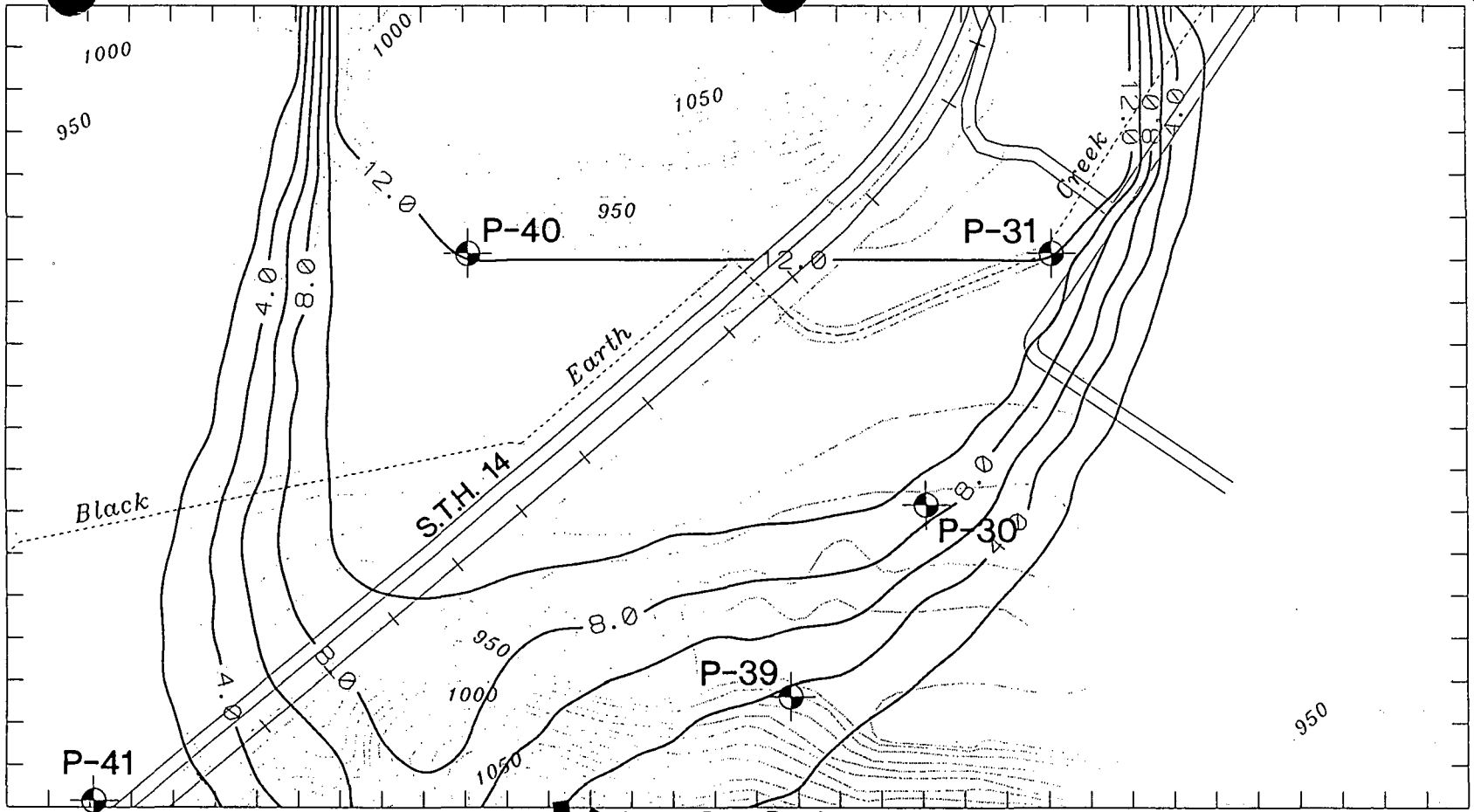REFUSE HIDEAWAY LANDFILL

**PROPOSED
SENTRY WELL LOCATION**

| PROJECT: 148E13673 | DATE: 12/03/91 | DRAWING NO.: 1367-c4s | FIGURE: 4-39 |

Table 3-1.   Hydraulic Conductivities Used to Calculate Average Model Hydraulic Conductivities

Location	Sand/Gravel Hydraulic Conductivity		Bedrock Hydraulic Conductivity	
	ft/sec.	cm/sec.	ft/sec.	cm/sec.
P-30I	1.3×10^{-3}	4.0×10^{-2}		
P-31IA	1.8×10^{-4}	5.6×10^{-3}		
P-31IB	7.7×10^{-4}	2.3×10^{-2}		
P-32S	1.0×10^{-4}	3.1×10^{-3}		
P-38S	2.2×10^{-5}	6.6×10^{-4}		
P-39S	3.0×10^{-4}	9.1×10^{-3}		
P-41D	2.5×10^{-4}	7.6×10^{-3}		
P-40D			7.2×10^{-5}*	2.2×10^{-3}*
P-30D			2.3×10^{-4}***	7.1×10^{-3}***
PRIVATE WELLS				
Sather			2.8×10^{-5}**	8.6×10^{-4}**
Sommers			4.7×10^{-6}**	1.4×10^{-4}**
Olson			1.8×10^{-5}**	5.6×10^{-4}**
Durand			8.3×10^{-5}**	2.5×10^{-3}**
Wilkowski			4.3×10^{-5}**	1.3×10^{-3}**
Rocky Dell Road			8.2×10^{-5}*	2.5×10^{-3}*
Rocky Dell Road			4.7×10^{-6}**	1.4×10^{-4}**
REFERENCES				
McLeod (1975)			8.3×10^{-5}*	2.5×10^{-3}*
McLeod (1975)			2.2×10^{-4}**	6.6×10^{-3}**
Cline (1965)			9.5×10^{-5} to 5.7×10^{-5}*	2.9×10^{-3} to 1.7×10^{-3}*

NOTE: *   Sandstone
            **   Dolomite/Sandstone
            ***   Dolomite

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Table 3-2   Comparison of Observed vs Model-Calibrated Hydraulic Heads

Monitor Well	Hydraulic Head (ft)		Difference (obs. - cal.)	Approximate Head Drop Across Cell (ft)
	Observed	Calibrated		
P-31IB	906.34	906.48	- .14	.11
P-40I	906.31	906.13	+ .18	.20
P-30I	905.84	905.85	- .01	.13
P-41D*	903.81	903.80	+ .01	.07

Notes:

*P-41 is located on a specified head boundary.

RMS error for P-31IB, P-40I, and P-30I is 0.13 feet.

Table 3-3 Model Permeability Values

Value	Initial Hydraulic Conductivities for Composite Transmissivity Calculations (ft/sec)		Composite Transmissivities (ft^2/sec)	Composite Hydraulic Conductivities Determined from Composite Transmissivities (ft/sec)
	Sand & Gravel	Bedrock		
Minimum			9.7×10^{-3}	3.9×10^{-5}
Maximum			4.9×10^{-2}	2.0×10^{-4}
Average	$4.2 \times 10^{-4}*$	$8.3 \times 10^{-5}*$	2.9×10^{-2}	1.2×10^{-4}
Standard Deviation			1.0×10^{-2}	4.0×10^{-5}

Note:

* Calculated from values presented in Table 3-1

Table 3-4 Measured Tetrachloroethylene Concentrations At Various Locations Through Time

Sampling Location	Tetrachloroethylene (PCE) Sampling Dates													
	5/90	6/90	7/90	8/90	9/90	10/90	11/90	12/90	1/91	4/91	6/91	7/91	10/91	11/91
Stoppleworth (private well)	12.4	11.3	8.6	9.2	8.1	19.1	12.2	12.8 and 11.2+		9.6		10.2	12	
Schultz (private well)								9.2		7.6		ND	9.2	
P-40I							12*	10	12		13			
P-31IB								14	11		13			
P-30I						ND*		ND	ND		ND			
P-41D							ND*	ND	ND			ND		
P-39								ND	ND					

Note: All concentrations in parts per billion

+ Two sampling events during that month
* Vertical profiling sample measurement

ND = Not detected

Table 3-5 Measured Trichloroethylene/1,2-Dichloroethylene Concentrations At Various Locations Through Time

Sampling Location	Trichloroethylene/1,2-Dichloroethylene Sampling Dates													
	5/90	6/90	7/90	8/90	9/90	10/90	11/90	12/90	1/91	4/91	6/91	7/91	10/91	11/91
Stoppleworth (private well)	2.7/7	2.2/5.3	2.7/4.3	1/5	1.1/3.7	2.4/9	2.2/6.4	2.1-2.2/5-7.1+		1.4/5.1		2.2/4.7	2.4/6.4	
Schultz (private well)								4.9/23.8		4.1/15.3		ND	4.6/16	
P-40I							2/1*	2/ND	2/ND		2/ND			
P-31IB								ND/ND	<2/ND		2/ND			
P-30I						ND/ND*		ND/ND	ND/ND		ND/ND			
P-41D							ND/ND*	ND/ND	ND/ND			ND/ND		
P-39								ND/ND	ND/ND					

Note: All concentration in parts per billion

+ Two sampling events during that month
* Vertical profiling sample measurement

ND = Not detected

TABLE 4-1. TIME PREDICTIONS FOR PCE DETECTIONS

MODELED CONDITIONS*		PCE DETECTION LOCATION			
		P-30	PRIVATE RESIDENCE[+]	P-41	COMMENTS
12 ppb Constant Source	Base Case K and degradation** (730-day ½-life)	ND	ND	ND →	Plume reaches equilibrium after approximately 5 years
		ND	ND	ND →	Plume reaches equilibrium after approximately 7.5 years
	Base Case K x 10 and degradation** (730-day ½-life)	ND	ND	ND →	Plume reaches equilibrium after approximately 5 years
		D (after 2.5 years)	D (after 5 years)	ND →	Plume reaches equilibrium after approximately 7.2 years
	Base Case K and no degradation	D (after 20 years)	D (after 40 years)	D (after 100 years) →	
	Base Case K x 10 and no degradation[++]	D (after 2.1 years)	D (after 4.1 years)	D (after 9 years) →	
12 ppb Source Removed at Time >0	Base Case K and degradation	ND	ND	ND →	All concentrations <1 ppb after 1.8 years
	Base Case K x 10 and degradation	ND	ND	ND →	All concentrations <1 ppb after 2.2 years
	Base Case K and no degradation	D (after 22 years)	D (after 45 years)	D (after 75 years) →	
	Base Case K x 10 and no degradation	D (after 2.2 years)	D (after 4.2 years)	D (after 10 years) →	

[+]   Closest Deer Run Subdivision home to the modeled area.

[++]   Most Conservative Modeled Scenario

*   All simulations above use 30 and 10 feet for sand and gravel and bedrock longitudinal dispersivity, respectively, and 25% and 5% for sand and gravel and bedrock effective porosity, respectively.

**   Conditions considered most representative of study site. Degradation (unless stated otherwise) is simulated as a 230-day ½-life.

ND   = No detection

D   = Detection >1 part per billion

APPENDIX A

MODEL DOCUMENTATION

APPENDIX A.1

MODFLOW DOCUMENTATION

```
C     ********************************************************************
C     MAIN CODE FOR MODULAR MODEL --    9/1/87
C           BY MICHAEL G. MCDONALD AND ARLEN W. HARBAUGH
C-----VERSION 1638 24JUL1987 MAIN1
C     ********************************************************************
C
C        SPECIFICATIONS:
C     ------------------------------------------------------------------
      COMMON X(30000)
      COMMON /FLWCOM/LAYCON(80)
      CHARACTER*4 HEADNG,VBNM
      DIMENSION HEADNG(32),VBNM(4,20),VBVL(4,20),IUNIT(24)
      DOUBLE PRECISION DUMMY
      EQUIVALENCE (DUMMY,X(1))
C     ------------------------------------------------------------------
C
C1------SET SIZE OF X ARRAY. REMEMBER TO REDIMENSION X.
      LENX=30000
C
C2------ASSIGN BASIC INPUT UNIT AND PRINTER UNIT.
      INBAS=1
      IOUT=6
C
C3------DEFINE PROBLEM__ROWS,COLUMNS,LAYERS,STRESS PERIODS,PACKAGES
      CALL BAS1DF(ISUM,HEADNG,NPER,ITMUNI,TOTIM,NCOL,NROW,NLAY,
     1               NODES,INBAS,IOUT,IUNIT)
C
C4------ALLOCATE SPACE IN "X" ARRAY.
      CALL BAS1AL(ISUM,LENX,LCHNEW,LCHOLD,LCIBOU,LCCR,LCCC,LCCV,
     1               LCHCOF,LCRHS,LCDELR,LCDELC,LCSTRT,LCBUFF,LCIOFL,
     2               INBAS,ISTRT,NCOL,NROW,NLAY,IOUT)
      IF(IUNIT(1).GT.0) CALL BCF1AL(ISUM,LENX,LCSC1,LCHY,
     1      LCBOT,LCTOP,LCSC2,LCTRPY,IUNIT(1),ISS,
     2      NCOL,NROW,NLAY,IOUT,IBCFCB)
      IF(IUNIT(2).GT.0) CALL WEL1AL(ISUM,LENX,LCWELL,MXWELL,NWELLS,
     1               IUNIT(2),IOUT,IWELCB)
      IF(IUNIT(3).GT.0) CALL DRN1AL(ISUM,LENX,LCDRAI,NDRAIN,MXDRN,
     1               IUNIT(3),IOUT,IDRNCB)
      IF(IUNIT(8).GT.0) CALL RCH1AL(ISUM,LENX,LCIRCH,LCRECH,NRCHOP,
     1           NCOL,NROW,IUNIT(8),IOUT,IRCHCB)
      IF(IUNIT(5).GT.0) CALL EVT1AL(ISUM,LENX,LCIEVT,LCEVTR,LCEXDP,
     1           LCSURF,NCOL,NROW,NEVTOP,IUNIT(5),IOUT,IEVTCB)
      IF(IUNIT(4).GT.0) CALL RIV1AL(ISUM,LENX,LCRIVR,MXRIVR,NRIVER,
     1           IUNIT(4),IOUT,IRIVCB)
      IF(IUNIT(7).GT.0) CALL GHB1AL(ISUM,LENX,LCBNDS,NBOUND,MXBND,
     1           IUNIT(7),IOUT,IGHBCB)
      IF(IUNIT(9).GT.0) CALL SIP1AL(ISUM,LENX,LCEL,LCFL,LCGL,LCV,
     1           LCHDCG,LCLRCH,LCW,MXITER,NPARM,NCOL,NROW,NLAY,
     2           IUNIT(9),IOUT)
      IF(IUNIT(11).GT.0) CALL SOR1AL(ISUM,LENX,LCA,LCRES,LCHDCG,LCLRCH,
     1           LCIEQP,MXITER,NCOL,NLAY,NSLICE,MBW,IUNIT(11),IOUT)
C
C5------IF THE "X" ARRAY IS NOT BIG ENOUGH THEN STOP.
      IF(ISUM-1.GT.LENX) STOP
C
C6------READ AND PREPARE INFORMATION FOR ENTIRE SIMULATION.
      CALL BAS1RP(X(LCIBOU),X(LCHNEW),X(LCSTRT),X(LCHOLD),
     1           ISTRT,INBAS,HEADNG,NCOL,NROW,NLAY,NODES,VBVL,X(LCIOFL),
     2           IUNIT(12),IHEDFM,IDDNFM,IHEDUN,IDDNUN,IOUT)
      IF(IUNIT(1).GT.0) CALL BCF1RP(X(LCIBOU),X(LCHNEW),X(LCSC1),
     1           X(LCHY),X(LCCR),X(LCCC),X(LCCV),X(LCDELR),
     2           X(LCDELC),X(LCBOT),X(LCTOP),X(LCSC2),X(LCTRPY),
     3           IUNIT(1),ISS,NCOL,NROW,NLAY,NODES,IOUT)
```

```
      IF(IUNIT(9).GT.0) CALL SIP1RP(NPARM,MXITER,ACCL,HCLOSE,X(LCW),
     1            IUNIT(9),IPCALC,IPRSIP,IOUT)
      IF(IUNIT(11).GT.0) CALL SOR1RP(MXITER,ACCL,HCLOSE,IUNIT(11),
     1            IPRSOR,IOUT)
C
C7------SIMULATE EACH STRESS PERIOD.
      DO 300 KPER=1,NPER
      KKPER=KPER
C
C7A-----READ STRESS PERIOD TIMING INFORMATION.
      CALL BAS1ST(NSTP,DELT,TSMULT,PERTIM,KKPER,INBAS,IOUT)
C
C7B-----READ AND PREPARE INFORMATION FOR STRESS PERIOD.
      IF(IUNIT(2).GT.0) CALL WEL1RP(X(LCWELL),NWELLS,MXWELL,IUNIT(2),
     1            IOUT)
      IF(IUNIT(3).GT.0) CALL DRN1RP(X(LCDRAI),NDRAIN,MXDRN,IUNIT(3),
     1            IOUT)
      IF(IUNIT(8).GT.0) CALL RCH1RP(NRCHOP,X(LCIRCH),X(LCRECH),
     1            X(LCDELR),X(LCDELC),NROW,NCOL,IUNIT(8),IOUT)
      IF(IUNIT(5).GT.0) CALL EVT1RP(NEVTOP,X(LCIEVT),X(LCEVTR),
     1            X(LCEXDP),X(LCSURF),X(LCDELR),X(LCDELC),NCOL,NROW,
     1            IUNIT(5),IOUT)
      IF(IUNIT(4).GT.0) CALL RIV1RP(X(LCRIVR),NRIVER,MXRIVR,IUNIT(4),
     1            IOUT)
      IF(IUNIT(7).GT.0) CALL GHB1RP(X(LCBNDS),NBOUND,MXBND,IUNIT(7),
     1            IOUT)
C
C7C-----SIMULATE EACH TIME STEP.
      DO 200 KSTP=1,NSTP
      KKSTP=KSTP
C
C7C1----CALCULATE TIME STEP LENGTH. SET HOLD=HNEW..
      CALL BAS1AD(DELT,TSMULT,TOTIM,PERTIM,X(LCHNEW),X(LCHOLD),KKSTP,
     1            NCOL,NROW,NLAY)
C
C7C2----ITERATIVELY FORMULATE AND SOLVE THE EQUATIONS.
      DO 100 KITER=1,MXITER
      KKITER=KITER
C
C7C2A---FORMULATE THE FINITE DIFFERENCE EQUATIONS.
      CALL BAS1FM(X(LCHCOF),X(LCRHS),NODES)
      IF(IUNIT(1).GT.0) CALL BCF1FM(X(LCHCOF),X(LCRHS),X(LCHOLD),
     1            X(LCSC1),X(LCHNEW),X(LCIBOU),X(LCCR),X(LCCC),X(LCCV),
     2            X(LCHY),X(LCTRPY),X(LCBOT),X(LCTOP),X(LCSC2),
     3            X(LCDELR),X(LCDELC),DELT,ISS,KKITER,KKSTP,KKPER,NCOL,
     4            NROW,NLAY,IOUT)
      IF(IUNIT(2).GT.0) CALL WEL1FM(NWELLS,MXWELL,X(LCRHS),X(LCWELL),
     1            X(LCIBOU),NCOL,NROW,NLAY)
      IF(IUNIT(3).GT.0) CALL DRN1FM(NDRAIN,MXDRN,X(LCDRAI),X(LCHNEW),
     1            X(LCHCOF),X(LCRHS),X(LCIBOU),NCOL,NROW,NLAY)
      IF(IUNIT(8).GT.0) CALL RCH1FM(NRCHOP,X(LCIRCH),X(LCRECH),
     1            X(LCRHS),X(LCIBOU),NCOL,NROW,NLAY)
      IF(IUNIT(5).GT.0) CALL EVT1FM(NEVTOP,X(LCIEVT),X(LCEVTR),
     1            X(LCEXDP),X(LCSURF),X(LCRHS),X(LCHCOF),X(LCIBOU),
     1            X(LCHNEW),NCOL,NROW,NLAY)
      IF(IUNIT(4).GT.0) CALL RIV1FM(NRIVER,MXRIVR,X(LCRIVR),X(LCHNEW),
     1            X(LCHCOF),X(LCRHS),X(LCIBOU),NCOL,NROW,NLAY)
      IF(IUNIT(7).GT.0) CALL GHB1FM(NBOUND,MXBND,X(LCBNDS),X(LCHCOF),
     1            X(LCRHS),X(LCIBOU),NCOL,NROW,NLAY)
C
```

```
C7C2B---MAKE ONE CUT AT AN APPROXIMATE SOLUTION.
      IF(IUNIT(9).GT.0) CALL SIP1AP(X(LCHNEW),X(LCIBOU),X(LCCR),X(LCCC),
     1     X(LCCV),X(LCHCOF),X(LCRHS),X(LCEL),X(LCFL),X(LCGL),X(LCV),
     2     X(LCW),X(LCHDCG),X(LCLRCH),NPARM,KKITER,HCLOSE,ACCL,ICNVG,
     3     KKSTP,KKPER,IPCALC,IPRSIP,MXITER,NSTP,NCOL,NROW,NLAY,NODES,
     4     IOUT)
      IF(IUNIT(11).GT.0) CALL SOR1AP(X(LCHNEW),X(LCIBOU),X(LCCR),
     1     X(LCCC),X(LCCV),X(LCHCOF),X(LCRHS),X(LCA),X(LCRES),X(LCIEQP),
     2     X(LCHDCG),X(LCLRCH),KKITER,HCLOSE,ACCL,ICNVG,KKSTP,KKPER,
     3     IPRSOR,MXITER,NSTP,NCOL,NROW,NLAY,NSLICE,MBW,IOUT)
C
C7C2C---IF CONVERGENCE CRITERION HAS BEEN MET STOP ITERATING.
      IF(ICNVG.EQ.1) GO TO 110
  100 CONTINUE
      KITER=MXITER
  110 CONTINUE
C
C7C3----DETERMINE WHICH OUTPUT IS NEEDED.
      CALL BAS1OC(NSTP,KKSTP,ICNVG,X(LCIOFL),NLAY,
     1 IBUDFL,ICBCFL,IHDDFL,IUNIT(12),IOUT)
C
C7C4----CALCULATE BUDGET TERMS. SAVE CELL-BY-CELL FLOW TERMS.
      MSUM=1
      IF(IUNIT(1).GT.0) CALL BCF1BD(VBNM,VBVL,MSUM,X(LCHNEW),
     1     X(LCIBOU),X(LCHOLD),X(LCSC1),X(LCCR),X(LCCC),X(LCCV),
     2     X(LCTOP),X(LCSC2),DELT,ISS,NCOL,NROW,NLAY,KKSTP,KKPER,
     3     IBCFCB,ICBCFL,X(LCBUFF),IOUT)
      IF(IUNIT(2).GT.0) CALL WEL1BD(NWELLS,MXWELL,VBNM,VBVL,MSUM,
     1     X(LCWELL),X(LCIBOU),DELT,NCOL,NROW,NLAY,KKSTP,KKPER,IWELCB,
     1     ICBCFL,X(LCBUFF),IOUT)
      IF(IUNIT(3).GT.0) CALL DRN1BD(NDRAIN,MXDRN,VBNM,VBVL,MSUM,
     1     X(LCDRAI),DELT,X(LCHNEW),NCOL,NROW,NLAY,X(LCIBOU),KKSTP,
     2     KKPER,IDRNCB,ICBCFL,X(LCBUFF),IOUT)
      IF(IUNIT(8).GT.0) CALL RCH1BD(NRCHOP,X(LCIRCH),X(LCRECH),
     1     X(LCIBOU),NROW,NCOL,NLAY,DELT,VBVL,VBNM,MSUM,KKSTP,KKPER,
     2     IRCHCB,ICBCFL,X(LCBUFF),IOUT)
      IF(IUNIT(5).GT.0) CALL EVT1BD(NEVTOP,X(LCIEVT),X(LCEVTR),
     1     X(LCEXDP),X(LCSURF),X(LCIBOU),X(LCHNEW),NCOL,NROW,NLAY,
     2     DELT,VBVL,VBNM,MSUM,KKSTP,KKPER,IEVTCB,ICBCFL,X(LCBUFF),IOUT)
      IF(IUNIT(4).GT.0) CALL RIV1BD(NRIVER,MXRIVR,X(LCRIVR),X(LCIBOU),
     1     X(LCHNEW),NCOL,NROW,NLAY,DELT,VBVL,VBNM,MSUM,
     2     KKSTP,KKPER,IRIVCB,ICBCFL,X(LCBUFF),IOUT)
      IF(IUNIT(7).GT.0) CALL GHB1BD(NBOUND,MXBND,VBNM,VBVL,MSUM,
     1     X(LCBNDS),DELT,X(LCHNEW),NCOL,NROW,NLAY,X(LCIBOU),KKSTP,
     2     KKPER,IGHBCB,ICBCFL,X(LCBUFF),IOUT)
C
C7C5---PRINT AND OR SAVE HEADS AND DRAWDOWNS. PRINT OVERALL BUDGET.
      CALL BAS1OT(X(LCHNEW),X(LCSTRT),ISTRT,X(LCBUFF),X(LCIOFL),
     1     MSUM,X(LCIBOU),VBNM,VBVL,KKSTP,KKPER,DELT,
     2     PERTIM,TOTIM,ITMUNI,NCOL,NROW,NLAY,ICNVG,
     3     IHDDFL,IBUDFL,IHEDFM,IHEDUN,IDDNFM,IDDNUN,IOUT)
C
C7C6----IF ITERATION FAILED TO CONVERGE THEN STOP.
      IF(ICNVG.EQ.0) STOP
  200 CONTINUE
  300 CONTINUE
C
C8------END PROGRAM
      STOP
C
      END
```

Module Documentation for the Basic Package

The Basic Package (BAS1) consists of eight primary modules and five submodules. The modules are:

Primary Modules

BAS1DF	Defines and sets key model parameters.
BAS1AL	Allocates space for data arrays used by the Basic Package.
BAS1RP	Reads and prepares data for the Basic Package.
BAS1ST	Reads timing information and initializes variables needed to calculate the length of time steps.
BAS1AD	Calculates the length of time steps, accumulates elapsed time, and intializes heads at the beginning of each time step.
BAS1FM	Clears accumulators RHS and HCOF.
BAS1OC	Sets flags which indicate when data should be printed or recorded on disk.
BAS1OT	Prints and records heads, drawdowns, and overall volumetric budget.

Submodules

SBAS1D	Calculates, writes, and records drawdown distribution.
SBAS1H	Writes and records head distribution.
SBAS1I	Initializes the Output Control System.
SBAS1T	Prints a time summary.
SBAS1V	Calculates and prints the overall volumetric budget.

```
      SUBROUTINE BAS1DF(ISUM,HEADNG,NPER,ITMUNI,TOTIM,NCOL,NROW,
     1      NLAY,NODES,INBAS,IOUT,IUNIT)
C
C-----VERSION 1513 12MAY1987 BAS1DF
C     ********************************************************************
C     DEFINE KEY MODEL PARAMETERS
C     ********************************************************************
C
C     SPECIFICATIONS:
C     ------------------------------------------------------------------
      CHARACTER*4 HEADNG
      DIMENSION HEADNG(32),IUNIT(24)
C     ------------------------------------------------------------------
C
C1------PRINT THE NAME OF THE PROGRAM.
      WRITE(IOUT,1)
    1 FORMAT(1H1,20X,'U.S. GEOLOGICAL SURVEY MODULAR',
     1        ' FINITE-DIFFERENCE GROUND-WATER MODEL')
C
C2------READ AND PRINT A HEADING.
      READ(INBAS,2) HEADNG
    2 FORMAT(20A4)
      WRITE(IOUT,3) HEADNG
    3 FORMAT(1H0,32A4)
C
C3------READ NUMBER OF LAYERS,ROWS,COLUMNS,STRESS PERIODS AND
C3------UNITS OF TIME CODE.
      READ(INBAS,4) NLAY,NROW,NCOL,NPER,ITMUNI
    4 FORMAT(8I10)
C
C4------PRINT # OF LAYERS, ROWS, COLUMNS AND STRESS PERIODS.
      WRITE(IOUT,5) NLAY,NROW,NCOL
    5 FORMAT(1X,I4,' LAYERS',I10,' ROWS',I10,' COLUMNS')
      WRITE(IOUT,6) NPER
    6 FORMAT(1X,I3,' STRESS PERIOD(S) IN SIMULATION')
C
C5------SELECT AND PRINT A MESSAGE SHOWING TIME UNITS.
      IF(ITMUNI.LT.0 .OR. ITMUNI.GT.5) ITMUNI=0
      GO TO (10,20,30,40,50),ITMUNI
      WRITE(IOUT,9)
    9 FORMAT(1X,'MODEL TIME UNITS ARE UNDEFINED')
      GO TO 100
   10 WRITE(IOUT,11)
   11 FORMAT(1X,'MODEL TIME UNIT IS SECONDS')
      GO TO 100
   20 WRITE(IOUT,21)
   21 FORMAT(1X,'MODEL TIME UNIT IS MINUTES')
      GO TO 100
   30 WRITE(IOUT,31)
   31 FORMAT(1X,'MODEL TIME UNIT IS HOURS')
      GO TO 100
   40 WRITE(IOUT,41)
   41 FORMAT(1X,'MODEL TIME UNIT IS DAYS')
      GO TO 100
   50 WRITE(IOUT,51)
   51 FORMAT(1X,'MODEL TIME UNIT IS YEARS')
C
C6------READ & PRINT INPUT UNIT NUMBERS (IUNIT) FOR MAJOR OPTIONS.
  100 READ(INBAS,101) IUNIT
  101 FORMAT(24I3)
      WRITE(IOUT,102) (I,I=1,24),IUNIT
  102 FORMAT(1H0,'I/O UNITS:'/1X,'ELEMENT OF IUNIT:',24I3,
     1                      /1X,'        I/O UNIT:',24I3)
C
C7------INITIALIZE TOAL ELAPSED TIME COUNTER STORAGE ARRAY COUNTER
C7------AND CALCULATE NUMBER OF CELLS.
      TOTIM=0.
      ISUM=1
      NODES=NCOL*NROW*NLAY
C
C8------RETURN
      RETURN
      END
```

```
          SUBROUTINE BAS1AL(ISUM,LENX,LCHNEW,LCHOLD,LCIBOU,LCCR,LCCC,LCCV,
     1               LCHCOF,LCRHS,LCDELR,LCDELC,LCSTRT,LCBUFF,LCIOFL,INBAS,
     1               ISTRT,NCOL,NROW,NLAY,IOUT)
C-----VERSION 1515 12MAY1987 BAS1AL
C     ******************************************************************
C     ALLOCATE SPACE FOR BASIC MODEL ARRAYS
C     ******************************************************************
C
C        SPECIFICATIONS:
C     ------------------------------------------------------------------
C     ------------------------------------------------------------------
C
C1------PRINT A MESSAGE IDENTIFYING THE PACKAGE.
      WRITE(IOUT,1)INBAS
    1 FORMAT(1H0,'BAS1 -- BASIC MODEL PACKAGE, VERSION 1, 9/1/87',
     2' INPUT READ FROM UNIT',I3)
C
C2------READ & PRINT FLAG IAPART (RHS & BUFFER SHARE SPACE?) AND
C2------FLAG ISTRT (SHOULD STARTING HEADS BE SAVED FOR DRAWDOWN?)
      READ(INBAS,2) IAPART,ISTRT
    2 FORMAT(2I10)
      IF(IAPART.EQ.0) WRITE(IOUT,3)
    3 FORMAT(1X,'ARRAYS RHS AND BUFF WILL SHARE MEMORY.')
      IF(ISTRT.NE.0) WRITE(IOUT,4)
    4 FORMAT(1X,'START HEAD WILL BE SAVED')
      IF(ISTRT.EQ.0) WRITE(IOUT,5)
    5 FORMAT(1X,'START HEAD WILL NOT BE SAVED',
     1      ' -- DRAWDOWN CANNOT BE CALCULATED')
C
C3------STORE,IN ISOLD, LOCATION OF FIRST UNALLOCATED SPACE IN X.
      ISOLD=ISUM
      NRCL=NROW*NCOL*NLAY
C
C4------ALLOCATE SPACE FOR ARRAYS.
      LCHNEW=ISUM
      ISUM=ISUM+2*NRCL
      LCHOLD=ISUM
      ISUM=ISUM+NRCL
      LCIBOU=ISUM
      ISUM=ISUM+NRCL
      LCCR=ISUM
      ISUM=ISUM+NRCL
      LCCC=ISUM
      ISUM=ISUM+NRCL
      LCCV=ISUM
      ISUM=ISUM+NROW*NCOL*(NLAY-1)
      LCHCOF=ISUM
      ISUM=ISUM+NRCL
      LCRHS=ISUM
      ISUM=ISUM+NRCL
      LCDELR=ISUM
      ISUM=ISUM+NCOL
      LCDELC=ISUM
      ISUM=ISUM+NROW
      LCIOFL=ISUM
      ISUM=ISUM+NLAY*4
C
C5------IF BUFFER AND RHS SHARE SPACE THEN LCBUFF=LCRHS.
      LCBUFF=LCRHS
      IF(IAPART.EQ.0) GO TO 50
      LCBUFF=ISUM
      ISUM=ISUM+NRCL
C
C6------IF STRT WILL BE SAVED THEN ALLOCATE SPACE.
   50 LCSTRT=ISUM
      IF(ISTRT.NE.0) ISUM=ISUM+NRCL
      ISP=ISUM-ISOLD
C
C7------PRINT AMOUNT OF SPACE USED.
      WRITE(IOUT,6) ISP
    6 FORMAT(1X,I8,' ELEMENTS IN X ARRAY ARE USED BY BAS')
      ISUM1=ISUM-1
      WRITE(IOUT,7) ISUM1,LENX
    7 FORMAT(1X,I8,' ELEMENTS OF X ARRAY USED OUT OF',I8)
      IF(ISUM1.GT.LENX) WRITE(IOUT,8)
    8 FORMAT(1X,'   ***X ARRAY MUST BE DIMENSIONED LARGER***')
C
C
C8------RETURN
      RETURN
C
      END
```

```
      SUBROUTINE BAS1RP(IBOUND,HNEW,STRT,HOLD,ISTRT,INBAS,
     1     HEADNG,NCOL,NROW,NLAY,NODES,VBVL,IOFLG,INOC,IHEDFM,
     2     IDDNFM,IHEDUN,IDDNUN,IOUT)
C-----VERSION 1628 15MAY1987 BAS1RP
C     *****************************************************************
C     READ AND INITIALIZE BASIC MODEL ARRAYS
C     *****************************************************************
C
C        SPECIFICATIONS:
C     ------------------------------------------------------------------
      CHARACTER*4 HEADNG,ANAME
      DOUBLE PRECISION HNEW,HNOFLO
C
      OIMENSION HNEW(NODES),IBOUND(NODES),STRT(NODES),HOLD(NODES),
     1                ANAME(6,2),VBVL(4,20),IOFLG(NLAY,4),HEADNG(32)
C
      DATA ANAME(1,1),ANAME(2,1),ANAME(3,1),ANAME(4,1),ANAME(5,1),
     1    ANAME(6,1) /'    ','    ','  BO','UNDA','RY A','RRAY'/
      DATA ANAME(1,2),ANAME(2,2),ANAME(3,2),ANAME(4,2),ANAME(5,2),
     1    ANAME(6,2) /'    ','    ','    ','INIT','IAL ','HEAD'/
C     ------------------------------------------------------------------
C
C1------PRINT SIMULATION TITLE, CALCULATE # OF CELLS IN A LAYER.
      WRITE(IOUT,1) HEADNG
    1 FORMAT(1H1,32A4)
      NCR=NCOL*NROW
C
C2------READ BOUNDARY ARRAY(IBOUND) ONE LAYER AT A TIME.
      DO 100 K=1,NLAY
      KK=K
      LOC=1+(K-1)*NCR
      CALL U2DINT(IBOUND(LOC),ANAME(1,1),NROW,NCOL,KK,INBAS,IOUT)
  100 CONTINUE
C
C3------READ AND PRINT HEAD VALUE TO BE PRINTED FOR NO-FLOW CELLS.
      READ(INBAS,2) TMP
    2 FORMAT(F10.0)
      HNOFLO=TMP
      WRITE(IOUT,3) TMP
    3 FORMAT(1H0,'AQUIFER HEAD WILL BE SET TO ',1PG11.5,
     1        ' AT ALL NO-FLOW NODES (IBOUND=0).')
C
C4------READ STARTING HEADS.
      DO 300 K=1,NLAY
      KK=K
      LOC=1+(K-1)*NCR
      CALL U2DREL(HOLD(LOC),ANAME(1,2),NROW,NCOL,KK,INBAS,IOUT)
  300 CONTINUE
C
C5------COPY INITIAL HEADS FROM HOLD TO HNEW.
      DO 400 I=1,NODES
      HNEW(I)=HOLD(I)
      IF(IBOUND(I).EQ.0) HNEW(I)=HNOFLO
  400 CONTINUE
C
C6------IF STARTING HEADS ARE TO BE SAVED THEN COPY HOLD TO STRT.
      IF(ISTRT.EQ.0) GO TO 590
      DO 500 I=1,NODES
      STRT(I)=HOLD(I)
  500 CONTINUE
C
C7------INITIALIZE VOLUMETRIC BUDGET ACCUMULATORS TO ZERO.
  590 DO 600 I=1,20
      DO 600 J=1,4
      VBVL(J,I)=0.
  600 CONTINUE
C
C8------SET UP OUTPUT CONTROL.
      CALL SBAS1I(NLAY,ISTRT,IOFLG,INOC,IOUT,IHEDFM,
     1           IDDNFM,IHEDUN,IDDNUN)
C
C9------RETURN
 1000 RETURN
      END
```

```
                  SUBROUTINE BAS1ST(NSTP,DELT,TSMULT,PERTIM,KPER,INBAS,IOUT)
      C
      C
      C-----VERSION 1614 08SEP1982 BAS1ST
      C     ****************************************************************
      C     SETUP TIME PARAMETERS FOR NEW TIME PERIOD
      C     ****************************************************************
      C
      C        SPECIFICATIONS:
      C     ----------------------------------------------------------------
      C     ----------------------------------------------------------------
      C
      C1------READ LENGTH OF STRESS PERIOD, NUMBER OF TIME STEPS AND.
      C1------TIME STEP MULTIPLIER.
            READ (INBAS,1) PERLEN,NSTP,TSMULT
          1 FORMAT(F10.0,I10,F10.0)
      C
      C2------CALCULATE THE LENGTH OF THE FIRST TIME STEP.
      C
      C2A-----ASSUME TIME STEP MULTIPLIER IS EQUAL TO ONE.
            DELT=PERLEN/FLOAT(NSTP)
      C
      C2B-----IF TIME STEP MULTIPLIER IS NOT ONE THEN CALCULATE FIRST
      C2B-----TERM OF GEOMETRIC PROGRESSION.
            IF(TSMULT.NE.1.) DELT=PERLEN*(1.-TSMULT)/(1.-TSMULT**NSTP)
      C
      C3------PRINT TIMING INFORMATION.
            WRITE (IOUT,2) KPER,PERLEN,NSTP,TSMULT,DELT
          2 FORMAT(1H1,51X,'STRESS PERIOD NO.',I4,', LENGTH =',G15.7/52X
           1,46('-')//52X,'NUMBER OF TIME STEPS =',I6
           2//53X,'MULTIPLIER FOR DELT =',F10.3
           3//50X,'INITIAL TIME STEP SIZE =',G15.7)
      C
      C4------INITIALIZE PERTIM (ELAPSED TIME WITHIN STRESS PERIOD).
            PERTIM=0.
      C
      C5------RETURN
            RETURN
            END
```

Module Documentation for the Block-Centered Flow Package

The Block-Centered Flow Package (BCF1) has four primary modules and three submodules. The relationship of the modules to MAIN and to each other is shown in figure 31. The flow of information used to calculate horizontal-hydraulic conductances (CC and CR) is shown for several of the modules. For example, BCF1RP passes transmissivity (T) and cell dimensions (DELR and DELC) to SBCF1N. Module SBCF1N then returns CC and CR to BCF1RP. The modules are:

Primary Modules

BCF1AL   Allocates space for data arrays.

BCF1RP   Reads all data needed by the package, invokes
           SBCF1N to reconcile input transmissive values
           with the IBOUND array, and calculates storage
           capacities and constant conductances.

BCF1FM   Calculates all coefficients of the system of
           equations that are not constant and invokes
           SBCF1H to calculate horizontal-branch conductances
           in partially saturated layers.

BCF1BD   Calculates flow rates and accumulated flow volumes
           into and out of storage and constant-head boundaries.
           When cell-by-cell flow is specified, flow across
           all sides of each cell is also calculated.

Submodules

SBCF1N   Reconciles input transmissive values with the IBOUND
           array and calculates storage capacities and constant
           conductances. Invokes SBCF1C to calculate horizontal-
           branch conductances for layers where transmissivity
           is constant.

SBCF1H   Calculates transmissivity for cells in layers where it
           depends on heads and invokes SBCF1C to calculate
           horizontal-branch conductances.

SBCF1C   Calculates horizontal-branch conductance from cell
           transmissivity.

SBCF1B   Calculates cell-by-cell flow terms across cell faces.

SBCF1F   Calculates flow terms (both cell-by-cell and entries
           to overall budget) for flow to and from constant-
           head cells.

```
      SUBROUTINE BAS1AD(DELT,TSMULT,TOTIM,PERTIM,HNEW,HOLD,KSTP,
     1                     NCOL,NROW,NLAY)
C
C-----VERSION 1412 22FEB1982 BAS1AD
C
C     ******************************************************************
C     ADVANCE TO NEXT TIME STEP
C     ******************************************************************
C
C        SPECIFICATIONS:
C     ------------------------------------------------------------------
      DOUBLE PRECISION HNEW
C
      DIMENSION HNEW(NCOL,NROW,NLAY), HOLD(NCOL,NROW,NLAY)
C     ------------------------------------------------------------------
C
C1------IF NOT FIRST TIME STEP THEN CALCULATE TIME STEP LENGTH.
      IF(KSTP.NE.1) DELT=TSMULT*DELT
C
C2------ACCUMULATE ELAPSED TIME IN SIMULATION(TOTIM) AND IN THIS
C2------STRESS PERIOD(PERTIM).
      TOTIM=TOTIM+DELT
      PERTIM=PERTIM+DELT
C
C3------COPY HNEW TO HOLD.
      DO 10 K=1,NLAY
      DO 10 I=1,NROW
      DO 10 J=1,NCOL
   10 HOLD(J,I,K)=HNEW(J,I,K)
C
C4------RETURN
      RETURN
      END
```

```fortran
      SUBROUTINE BAS1FM(HCOF,RHS,NODES)
C
C
C-----VERSION 1632 24JUL1987 BAS1FM
C     ******************************************************************
C     SET HCOF=RHS=0.
C     ******************************************************************
C
C        SPECIFICATIONS:
C     -----------------------------------------------------------------
      DIMENSION HCOF(NODES),RHS(NODES)
C     -----------------------------------------------------------------
C
C1------FOR EACH CELL INITIALIZE HCOF AND RHS ACCUMULATORS.
      DO 100 I=1,NODES
      HCOF(I)=0.
      RHS(I)=0.
  100 CONTINUE
C
C2------RETURN
      RETURN
      END
```

```
      SUBROUTINE BAS1OC(NSTP,KSTP,ICNVG,IOFLG,NLAY,
     1      IBUDFL,ICBCFL,IHDDFL,INOC,IOUT)
C
C-----VERSION 1632 24JUL1987 BAS1OC
C     ********************************************************************
C     OUTPUT CONTROLLER FOR HEAD, DRAWDOWN, AND BUDGET
C     ********************************************************************
C
C        SPECIFICATIONS:
C     ------------------------------------------------------------------
      DIMENSION IOFLG(NLAY,4)
C     ------------------------------------------------------------------
C
C
C1------TEST UNIT NUMBER (INOC (INOC=IUNIT(12))) TO SEE IF
C1------OUTPUT CONTROL IS ACTIVE.
      IF(INOC.NE.0)GO TO 500
C
C2------IF OUTPUT CONTROL IS INACTIVE THEN SET DEFAULTS AND RETURN.
      IHDDFL=0
      IF(ICNVG.EQ.0 .OR. KSTP.EQ.NSTP)IHDDFL=1
      IBUDFL=0
      IF(ICNVG.EQ.0 .OR. KSTP.EQ.NSTP)IBUDFL=1
      ICBCFL=0
      GO TO 1000
C
C3-------READ AND PRINT OUTPUT FLAGS AND CODE FOR DEFINING IOFLG.
  500 READ(INOC,1) INCODE,IHDDFL,IBUDFL,ICBCFL
    1 FORMAT(4I10)
      WRITE(IOUT,3) IHDDFL,IBUDFL,ICBCFL
    3 FORMAT(1H0,'HEAD/DRAWDOWN PRINTOUT FLAG =',I2,
     1    5X,'TOTAL BUDGET PRINTOUT FLAG =',I2,
     2    5X,'CELL-BY-CELL FLOW TERM FLAG =',I2)
C
C4------DECODE INCODE TO DETERMINE HOW TO SET FLAGS IN IOFLG.
      IF(INCODE) 100,200,300
C
C5------USE IOFLG FROM LAST TIME STEP.
  100 WRITE(IOUT,101)
  101 FORMAT(1H ,'REUSING PREVIOUS VALUES OF IOFLG')
      GO TO 600
C
C6------READ IOFLG FOR LAYER 1 AND ASSIGN SAME TO ALL LAYERS
  200 READ(INOC,201) (IOFLG(1,M),M=1,4)
  201 FORMAT(4I10)
      DO 210 K=1,NLAY
      IOFLG(K,1)=IOFLG(1,1)
      IOFLG(K,2)=IOFLG(1,2)
      IOFLG(K,3)=IOFLG(1,3)
      IOFLG(K,4)=IOFLG(1,4)
  210 CONTINUE
      WRITE(IOUT,211) (IOFLG(1,M),M=1,4)
  211 FORMAT(1H0,'OUTPUT FLAGS FOR ALL LAYERS ARE THE SAME:'/
     1    1X,'  HEAD    DRAWDOWN HEAD   DRAWDOWN'/
     2    1X,'PRINTOUT PRINTOUT SAVE     SAVE'/
     3    1X,34('-')/1X,I5,I10,I8,I8)
      GO TO 600
C
C7------READ IOFLG IN ENTIRETY
  300 READ(INOC,301) ((IOFLG(K,I),I=1,4),K=1,NLAY)
  301 FORMAT(4I10)
      WRITE(IOUT,302)
  302 FORMAT(1H0,'OUTPUT FLAGS FOR EACH LAYER:'/
     1    1X,'         HEAD    DRAWDOWN HEAD   DRAWDOWN'/
     2    1X,'LAYER PRINTOUT PRINTOUT SAVE     SAVE'/
     3    1X,41('-'))
      WRITE(IOUT,303) (K,(IOFLG(K,I),I=1,4),K=1,NLAY)
  303 FORMAT(1X,I4,I8,I10,I8,I8)
C
C8------THE LAST STEP IN A STRESS PERIOD AND STEPS WHERE ITERATIVE
C8------PROCEDURE FAILED TO CONVERGE GET A VOLUMETRIC BUDGET.
  600 IF(ICNVG.EQ.0 .OR. KSTP.EQ.NSTP) IBUDFL=1
C
C9------RETURN
 1000 RETURN
      END
```

```
          SUBROUTINE BAS1OT(HNEW,STRT,ISTRT,BUFF,IOFLG,MSUM,IBOUND,VBNM,
       1  VBVL,KSTP,KPER,DELT,PERTIM,TOTIM,ITMUNI,NCOL,NROW,NLAY,ICNVG,
       2  IHDDFL,IBUDFL,IHEDFM,IHEDUN,IDDNFM,IDDNUN,IOUT)
C-----VERSION 1522 12MAY1987 BAS1OT
C     ******************************************************************
C     OUTPUT TIME, VOLUMETRIC BUDGET, HEAD, AND DRAWDOWN
C     ******************************************************************
C
C        SPECIFICATIONS:
C     ------------------------------------------------------------------
      CHARACTER*4 VBNM
      DOUBLE PRECISION HNEW
C
      DIMENSION HNEW(NCOL,NROW,NLAY),STRT(NCOL,NROW,NLAY),
     1          VBNM(4,20),VBVL(4,20),IOFLG(NLAY,4),
     2          IBOUND(NCOL,NROW,NLAY),BUFF(NCOL,NROW,NLAY)
C     ------------------------------------------------------------------
C
C1------CLEAR PRINTOUT FLAG (IPFLG)
      IPFLG=0
C
C2------IF ITERATIVE PROCEDURE FAILED TO CONVERGE PRINT MESSAGE
      IF(ICNVG.EQ.0) WRITE(IOUT,1) KSTP,KPER
    1 FORMAT(1H0,10X,'****FAILED TO CONVERGE IN TIME STEP',I3,
     1      ' OF STRESS PERIOD',I3,'****')
C
C3------IF HEAD AND DRAWDOWN FLAG (IHDDFL) IS SET WRITE HEAD AND
C3------DRAWDOWN IN ACCORDANCE WITH FLAGS IN IOFLG.
      IF(IHDDFL.EQ.0) GO TO 100
C
      CALL SBAS1H(HNEW,BUFF,IOFLG,KSTP,KPER,NCOL,NROW,
     1     NLAY,IOUT,IHEDFM,IHEDUN,IPFLG,PERTIM,TOTIM)
      CALL SBAS1D(HNEW,BUFF,IOFLG,KSTP,KPER,NCOL,NROW,NLAY,IOUT,
     1 IDDNFM,IDDNUN,STRT,ISTRT,IBOUND,IPFLG,PERTIM,TOTIM)
C
C4------PRINT TOTAL BUDGET IF REQUESTED
  100 IF(IBUDFL.EQ.0) GO TO 120
      CALL SBAS1V(MSUM,VBNM,VBVL,KSTP,KPER,IOUT)
      IPFLG=1
C
C5------END PRINTOUT WITH TIME SUMMARY AND FORM FEED IF ANY PRINTOUT
C5------WILL BE PRODUCED.
  120 IF(IPFLG.EQ.0) RETURN
      CALL SBAS1T(KSTP,KPER,DELT,PERTIM,TOTIM,ITMUNI,IOUT)
      WRITE(IOUT,101)
  101 FORMAT(1H1)
C
C6------RETURN
      RETURN
      END
```

```
      SUBROUTINE SBAS1D(HNEW,BUFF,IOFLG,KSTP,KPER,NCOL,NROW,
     1    NLAY,IOUT,IDDNFM,IDDNUN,STRT,ISTRT,IBOUND,IPFLG,
     2    PERTIM,TOTIM)
C-----VERSION 1630 15MAY1987 SBAS1D
C     ************************************************************
C     CALCULATE PRINT AND RECORD DRAWDOWNS
C     ************************************************************
C
C     SPECIFICATIONS
C     ------------------------------------------------------------
      CHARACTER*4 TEXT
      DOUBLE PRECISION HNEW
C
      DIMENSION HNEW(NCOL,NROW,NLAY),IOFLG(NLAY,4),TEXT(4),
     1    BUFF(NCOL,NROW,NLAY),STRT(NCOL,NROW,NLAY),
     2    IBOUND(NCOL,NROW,NLAY)
C
      DATA TEXT(1),TEXT(2),TEXT(3),TEXT(4) /'    ','    ','DRAW',
     1        'DOWN'/
C     ------------------------------------------------------------
C
C1------FOR EACH LAYER CALCULATE DRAWDOWN IF PRINT OR RECORD
C1------IS REQUESTED
      DO 59 K=1,NLAY
C
C2------IS DRAWDOWN NEEDED FRO THIS LAYER?
      IF(IOFLG(K,2).EQ.0 .AND. IOFLG(K,4).EQ.0) GO TO 59
C
C3------DRAWDOWN IS NEEDED. WERE STARTING HEADS SAVED?
      IF(ISTRT.NE.0) GO TO 53
C
C4------STARTING HEADS WERE NOT SAVED. PRINT MESSAGE AND STOP.
      WRITE(IOUT,52)
   52 FORMAT(1H0,'CANNOT CALCULATE DRAWDOWN BECAUSE START',
     1   ' HEADS WERE NOT SAVED')
      STOP
C
C5------CALCULATE DRAWDOWN FOR THE LAYER.
   53 DO 58 I=1,NROW
      DO 58 J=1,NCOL
      HSING=HNEW(J,I,K)
      BUFF(J,I,K)=HSING
      IF(IBOUND(J,I,K).NE.0) BUFF(J,I,K)=STRT(J,I,K)-HSING
   58 CONTINUE
   59 CONTINUE
C
C6------FOR EACH LAYER: DETERMINE IF DRAWDOWN SHOULD BE PRINTED.
C6------IF SO THEN CALL ULAPRS OR ULAPRW TO PRINT DRAWDOWN.
      DO 69 K=1,NLAY
      KK=K
      IF(IOFLG(K,2).EQ.0) GO TO 69
      IF(IDDNFM.LT.0) CALL ULAPRS(BUFF(1,1,K),TEXT(1),KSTP,KPER,
     1           NCOL,NROW,KK,-IDDNFM,IOUT)
      IF(IDDNFM.GE.0) CALL ULAPRW(BUFF(1,1,K),TEXT(1),KSTP,KPER,
     1           NCOL,NROW,KK,IDDNFM,IOUT)
      IPFLG=1
   69 CONTINUE
C
C7------FOR EACH LAYER: DETERMINE IF DRAWDOWN SHOULD BE RECORDED.
C7------IF SO THEN CALL ULASAV TO RECORD DRAWDOWN.
      IFIRST=1
      IF(IDDNUN.LE.0) GO TO 80
      DO 79 K=1,NLAY
      KK=K
      IF(IOFLG(K,4).LE.0) GO TO 79
      IF(IFIRST.EQ.1) WRITE(IOUT,74) IDDNUN,KSTP,KPER
   74 FORMAT(1H0,'DRAWDOWN WILL BE SAVED ON UNIT',I3,
     1   ' AT END OF TIME STEP',I3,', STRESS PERIOD',I3)
      IFIRST=0
      CALL ULASAV(BUFF(1,1,K),TEXT(1),KSTP,KPER,PERTIM,TOTIM,NCOL,
     1           NROW,KK,IDDNUN)
   79 CONTINUE
C
C8------RETURN
   80 RETURN
      END
```

```
      SUBROUTINE SBAS1H(HNEW,BUFF,IOFLG,KSTP,KPER,NCOL,NROW,
     1      NLAY,IOUT,IHEDFM,IHEDUN,IPFLG,PERTIM,TOTIM)
C
C-----VERSION 1653 15MAY1987 SBAS1H
C     ************************************************************
C     PRINT AND RECORD HEADS
C     ************************************************************
C
C        SPECIFICATIONS
C     ------------------------------------------------------------
      CHARACTER*4 TEXT
      DOUBLE PRECISION HNEW
C
      DIMENSION HNEW(NCOL,NROW,NLAY),IOFLG(NLAY,4),TEXT(4),
     1      BUFF(NCOL,NROW,NLAY)
C
      DATA TEXT(1),TEXT(2),TEXT(3),TEXT(4) /'    ','    ','    ',
     1      'HEAD'/
C     ------------------------------------------------------------
C
C1------FOR EACH LAYER: PRINT HEAD IF REQUESTED.
      DO 39 K=1,NLAY
      KK=K
C
C2------TEST IOFLG TO SEE IF HEAD SHOULD BE PRINTED.
      IF(IOFLG(K,1).EQ.0) GO TO 39
      IPFLG=1
C
C3------COPY HEADS FOR THIS LAYER INTO BUFFER.
      DO 32 I=1,NROW
      DO 32 J=1,NCOL
      BUFF(J,I,1)=HNEW(J,I,K)
   32 CONTINUE
C
C4------CALL UTILITY MODULE TO PRINT CONTENTS OF BUFFER.
      IF(IHEDFM.LT.0) CALL ULAPRS(BUFF,TEXT(1),KSTP,KPER,NCOL,NROW,KK,
     1           -IHEDFM,IOUT)
      IF(IHEDFM.GE.0) CALL ULAPRW(BUFF,TEXT(1),KSTP,KPER,NCOL,NROW,KK,
     1            IHEDFM,IOUT)
   39 CONTINUE
C
C5------IF UNIT FOR RECORDING HEADS <= 0: THEN RETURN.
      IF(IHEDUN.LE.0)GO TO 50
      IFIRST=1
C
C6------FOR EACH LAYER: RECORD HEAD IF REQUESTED.
      DO 49 K=1,NLAY
      KK=K
C
C7------CHECK IOFLG TO SEE IF HEAD FOR THIS LAYER SHOULD BE RECORDED.
      IF(IOFLG(K,3).LE.0) GO TO 49
      IF(IFIRST.EQ.1) WRITE(IOUT,41) IHEDUN,KSTP,KPER
   41 FORMAT(1H0,'HEAD WILL BE SAVED ON UNIT',I3,' AT END OF TIME STEP',
     1    I3,', STRESS PERIOD',I3)
      IFIRST=0
C
C8------COPY HEADS FOR THIS LAYER INTO BUFFER.
      DO 44 I=1,NROW
      DO 44 J=1,NCOL
      BUFF(J,I,1)=HNEW(J,I,K)
   44 CONTINUE
C
C9------RECORD CONTENTS OF BUFFER ON UNIT=IHEDUN
      CALL ULASAV(BUFF,TEXT(1),KSTP,KPER,PERTIM,TOTIM,NCOL,NROW,KK,
     1            IHEDUN)
   49 CONTINUE
C
C10-----RETURN
   50 RETURN
      END
```

```
      SUBROUTINE SBAS1I(NLAY,ISTRT,IOFLG,INOC,IOUT,IHEDFM,
     1             IDDNFM,IHEDUN,IDDNUN)
C
C-----VERSION 1531 12MAY1987 SBAS1I
C     ****************************************************************
C     SET UP OUTPUT CONTROL
C     ****************************************************************
C
C     SPECIFICATIONS:
C     ----------------------------------------------------------------
      DIMENSION IOFLG(NLAY,4)
C     ----------------------------------------------------------------
C
C1------TEST UNIT NUMBER FROM IUNIT (INOC) TO SEE IF OUTPUT
C1------CONTROL IS ACTIVE.
      IF(INOC.LE.0) GO TO 600
C
C2------READ AND PRINT FORMATS FOR PRINTING AND UNIT NUMBERS FOR
C2------RECORDING HEADS AND DRAWDOWN. THEN RETURN.
  500 READ (INOC,1)IHEDFM,IDDNFM,IHEDUN,IDDNUN
    1 FORMAT (4I10)
      WRITE (IOUT,3)IHEDFM,IDDNFM
    3 FORMAT (1H0,'HEAD PRINT FORMAT IS FORMAT NUMBER',I4,
     1         '    DRAWDOWN PRINT FORMAT IS FORMAT NUMBER',I4)
      WRITE (IOUT,4)IHEDUN,IDDNUN
    4 FORMAT (1H0,'HEADS WILL BE SAVED ON UNIT',I3,
     1         '    DRAWDOWNS WILL BE SAVED ON UNIT',I3)
      WRITE(IOUT,561)
  561 FORMAT(1H0,'OUTPUT CONTROL IS SPECIFIED EVERY TIME STEP')
      GO TO 1000
C
C3------OUTPUT CONTROL IS INACTIVE. PRINT A MESSAGE LISTING DEFAULTS.
  600 WRITE(IOUT,641)
  641 FORMAT(1H0,'DEFAULT OUTPUT CONTROL -- THE FOLLOWING OUTPUT',
     1         ' COMES AT THE END OF EACH STRESS PERIOD:')
      WRITE(IOUT,642)
  642 FORMAT(1X,'TOTAL VOLUMETRIC BUDGET')
      WRITE(IOUT,643)
  643 FORMAT(1X,10X,'HEAD')
      IF(ISTRT.NE.0)WRITE(IOUT,644)
  644 FORMAT(1X,10X,'DRAWDOWN')
C
C4------SET THE FORMAT CODES EQUAL TO THE DEFAULT FORMAT.
      IHEDFM=0
      IDDNFM=0
C
C5------SET DEFAULT FLAGS IN IOFLG SO THAT HEAD (AND DRAWDOWN) IS
C5------PRINTED FOR EVERY LAYER.
      ID=0
      IF(ISTRT.NE.0) ID=1
  670 DO 680 K=1,NLAY
      IOFLG(K,1)=1
      IOFLG(K,2)=ID
      IOFLG(K,3)=0
      IOFLG(K,4)=0
  680 CONTINUE
      GO TO 1000
C
C6------RETURN
 1000 RETURN
      END
```

```
         SUBROUTINE SBAS1T(KSTP,KPER,DELT,PERTIM,TOTIM,ITMUNI,IOUT)
C
C
C-----VERSION 0837 09APR1982 SBAS1T
C     *****************************************************************
C     PRINT SIMULATION TIME
C     *****************************************************************
C
C         SPECIFICATIONS:
C     -----------------------------------------------------------------
C     -----------------------------------------------------------------
      WRITE(IOUT,199) KSTP,KPER
  199 FORMAT(1H0,///10X,'TIME SUMMARY AT END OF TIME STEP',I3,
     1      ' IN STRESS PERIOD',I3)
C
C1------USE TIME UNIT INDICATOR TO GET FACTOR TO CONVERT TO SECONDS.
      CNV=0.
      IF(ITMUNI.EQ.1) CNV=1.
      IF(ITMUNI.EQ.2) CNV=60.
      IF(ITMUNI.EQ.3) CNV=3600.
      IF(ITMUNI.EQ.4) CNV=86400.
      IF(ITMUNI.EQ.5) CNV=31557600.
C
C2------IF FACTOR=0 THEN TIME UNITS ARE NON-STANDARD.
      IF(CNV.NE.0.) GO TO 100
C
C2A-----PRINT TIMES IN NON-STANDARD TIME UNITS.
      WRITE(IOUT,301) DELT,PERTIM,TOTIM
  301 FORMAT(21X,'     TIME STEP LENGTH =',G15.6/
     1       21X,'    STRESS PERIOD TIME =',G15.6/
     2       21X,'TOTAL SIMULATION TIME =',G15.6)
C
C2B-----RETURN
      RETURN
C
C3------CALCULATE LENGTH OF TIME STEP & ELAPSED TIMES IN SECONDS.
  100 DELSEC=CNV*DELT
      TOTSEC=CNV*TOTIM
      PERSEC=CNV*PERTIM
C
C4------CALCULATE TIMES IN MINUTES,HOURS,DAYS AND YEARS.
      DELMN=DELSEC/60.
      DELHR=DELMN/60.
      DELDY=DELHR/24.
      DELYR=DELDY/365.25
      TOTMN=TOTSEC/60.
      TOTHR=TOTMN/60.
      TOTDY=TOTHR/24.
      TOTYR=TOTDY/365.25
      PERMN=PERSEC/60.
      PERHR=PERMN/60.
      PERDY=PERHR/24.
      PERYR=PERDY/365.25
C
C5------PRINT TIME STEP LENGTH AND ELAPSED TIMES IN ALL TIME UNITS.
      WRITE(IOUT,200)
  200 FORMAT(27X,'   SECONDS         MINUTES            HOURS',10X,
     1       'DAYS            YEARS'/27X,75('-'))
      WRITE (IOUT,201) DELSEC,DELMN,DELHR,DELDY,DELYR
  201 FORMAT(1X,'     TIME STEP LENGTH',5X,5G15.6)
      WRITE(IOUT,202) PERSEC,PERMN,PERHR,PERDY,PERYR
  202 FORMAT(1X,'   STRESS PERIOD TIME',5X,5G15.6)
      WRITE(IOUT,203) TOTSEC,TOTMN,TOTHR,TOTDY,TOTYR
  203 FORMAT(1X,'TOTAL SIMULATION TIME',5X,5G15.6)
C
C6------RETURN
      RETURN
      END
```

```
      SUBROUTINE SBAS1V(MSUM,VBNM,VBVL,KSTP,KPER,IOUT)
C
C
C-----VERSION 1531 12MAY1987 SBAS1V
C     ******************************************************************
C     PRINT VOLUMETRIC BUDGET
C     ******************************************************************
C
C     SPECIFICATIONS:
C     ------------------------------------------------------------------
      CHARACTER*4 VBNM
      DIMENSION VBNM(4,20),VBVL(4,20)
C     ------------------------------------------------------------------
C
C1------DETERMINE NUMBER OF INDIVIDUAL BUDGET ENTRIES.
      MSUM1=MSUM-1
      IF(MSUM1.LE.0) RETURN
C
C2------CLEAR RATE AND VOLUME ACCUMULATORS.
      TOTRIN=0.
      TOTROT=0.
      TOTVIN=0.
      TOTVOT=0.
C
C3------ADD RATES AND VOLUMES (IN AND OUT) TO ACCUMULATORS.
      DO 100 L=1,MSUM1
      TOTRIN=TOTRIN+VBVL(3,L)
      TOTROT=TOTROT+VBVL(4,L)
      TOTVIN=TOTVIN+VBVL(1,L)
      TOTVOT=TOTVOT+VBVL(2,L)
  100 CONTINUE
C
C4------PRINT TIME STEP NUMBER AND STRESS PERIOD NUMBER.
      WRITE(IOUT,260) KSTP,KPER
      WRITE(IOUT,265)
C
C5------PRINT INDIVIDUAL INFLOW RATES AND VOLUMES AND THEIR TOTALS.
      DO 200 L=1,MSUM1
      WRITE(IOUT,275) (VBNM(I,L),I=1,4),VBVL(1,L),(VBNM(I,L),I=1,4)
     1,VBVL(3,L)
  200 CONTINUE
      WRITE(IOUT,286) TOTVIN,TOTRIN
C
C6------PRINT INDIVIDUAL OUTFLOW RATES AND VOLUMES AND THEIR TOTALS.
      WRITE(IOUT,287)
      DO 250 L=1,MSUM1
```

```
            WRITE(IOUT,275) (VBNM(I,L),I=1,4),VBVL(2,L),(VBNM(I,L),I=1,4)
           1,VBVL(4,L)
       250 CONTINUE
            WRITE(IOUT,298) TOTVOT,TOTROT
C
C7------CALCULATE THE DIFFERENCE BETWEEN INFLOW AND OUTFLOW.
C
C7A-----CALCULATE DIFFERENCE BETWEEN RATE IN AND RATE OUT.
            DIFFR=TOTRIN-TOTROT
C
C7B-----CALCULATE PERCENT DIFFERENCE BETWEEN RATE IN AND RATE OUT.
            PDIFFR=100.*DIFFR/((TOTRIN+TOTROT)/2)
C
C7C-----CALCULATE DIFFERENCE BETWEEN VOLUME IN AND VOLUME OUT.
            DIFFV=TOTVIN-TOTVOT
C
C7D-----GET PERCENT DIFFERENCE BETWEEN VOLUME IN AND VOLUME OUT.
            PDIFFV=100.*DIFFV/((TOTVIN+TOTVOT)/2)
C
C8------PRINT DIFFERENCES AND PERCENT DIFFERENCES BETWEEN INPUT
C8------AND OUTPUT RATES AND VOLUMES.
            WRITE(IOUT,299) DIFFV,DIFFR
            WRITE(IOUT,300) PDIFFV,PDIFFR
C
C9------RETURN
            RETURN
C
C     ---FORMATS
C
       260 FORMAT(1H0,///30X,'VOLUMETRIC BUDGET FOR ENTIRE MODEL AT END OF'
           1,' TIME STEP',I3,' IN STRESS PERIOD',I3/30X,77('-'))
       265 FORMAT(1H0,19X,'CUMULATIVE VOLUMES',6X,'L**3',37X
           1,'RATES FOR THIS TIME STEP',6X,'L**3/T'/20X,18('-'),47X,24('-')
           2//26X,'IN:',68X,'IN:'/26X,'---',68X,'---')
       275 FORMAT(1X,18X,4A4,' =',G14.5,39X,4A4,' =',G14.5)
       286 FORMAT(1H0,26X,'TOTAL IN =',G14.5,47X,'TOTAL IN ='
           1,G14.5)
       287 FORMAT(1H0,24X,'OUT:',67X,'OUT:'/25X,4('-'),67X,4('-'))
       298 FORMAT(1H0,25X,'TOTAL OUT =',G14.5,46X,'TOTAL OUT ='
           1,G14.5)
       299 FORMAT(1H0,26X,'IN - OUT =',G14.5,47X,'IN - OUT =',G14.5)
       300 FORMAT(1H0,15X,'PERCENT DISCREPANCY =',F20.2
           1,30X,'PERCENT DISCREPANCY =',F20.2,///)
C
            END
```

```
      SUBROUTINE BCF1AL(ISUM,LENX,LCSC1,LCHY,LCBOT,
     1      LCTOP,LCSC2,LCTRPY,IN,ISS,NCOL,NROW,NLAY,IOUT,IBCFCB)
C
C-----VERSION 1542 12MAY1987 BCF1AL
C
C     ******************************************************************
C     ALLOCATE ARRAY STORAGE FOR BLOCK-CENTERED FLOW PACKAGE
C     ******************************************************************
C
C        SPECIFICATIONS:
C     ------------------------------------------------------------------
      COMMON /FLWCOM/LAYCON(80)
C     ------------------------------------------------------------------
C
C1------IDENTIFY PACKAGE
      WRITE(IOUT,1)IN
    1 FORMAT(1H0,'BCF1 -- BLOCK-CENTERED FLOW PACKAGE, VERSION 1',
     1', 9/1/87',' INPUT READ FROM UNIT',I3)
C
C2------READ AND PRINT ISS (STEADY-STATE FLAG) AND IBCFCB (FLAG FOR
C2------PRINTING OR UNIT# FOR RECORDING CELL-BY-CELL FLOW TERMS)
      READ(IN,2) ISS,IBCFCB
    2 FORMAT(2I10)
      IF(ISS.EQ.0) WRITE(IOUT,3)
    3 FORMAT(1X,'TRANSIENT SIMULATION')
      IF(ISS.NE.0) WRITE(IOUT,4)
    4 FORMAT(1X,'STEADY-STATE SIMULATION')
      IF(IBCFCB.GT.0) WRITE(IOUT,9) IBCFCB
    9 FORMAT(1X,'CELL-BY-CELL FLOWS WILL BE RECORDED ON UNIT',I3)
      IF(IBCFCB.LT.0) WRITE(IOUT,88)
   88 FORMAT(1X,'CONSTANT HEAD CELL-BY-CELL FLOWS WILL BE PRINTED')
C
C3------READ TYPE CODE FOR EACH LAYER AND COUNT TOPS AND BOTTOMS
      IF(NLAY.LE.80) GO TO 50
      WRITE(IOUT,11)
   11 FORMAT(1H0,'YOU HAVE SPECIFIED MORE THAN 80 MODEL LAYERS'/1X,
     1  'SPACE IS RESERVED FOR A MAXIMUM OF 80 LAYERS IN ARRAY LAYCON')
      STOP
C
C3A-----READ LAYER TYPE CODES.
   50 READ(IN,51) (LAYCON(I),I=1,NLAY)
   51 FORMAT(40I2)
C           BOTTOM IS READ FOR TYPES 1,3    TOP IS READ FOR TYPES 2,3
      WRITE(IOUT,52)
   52 FORMAT(1X,5X,'LAYER  AQUIFER TYPE',/1X,5X,19('-'))
C
C3B-----INITIALIZE TOP AND BOTTOM COUNTERS.
      NBOT=0
      NTOP=0
C
C3C------PRINT LAYER TYPE AND COUNT TOPS AND BOTTOMS NEEDED.
      DO 100 I=1,NLAY
C
```

```
C3C1----PRINT LAYER NUMBER AND LAYER TYPE CODE.
      L=LAYCON(I)
      WRITE(IOUT,7) I,L
    7 FORMAT(1X,I9,I10)
C
C3C2----ONLY THE TOP LAYER CAN BE UNCONFINED(LAYCON=1).
      IF(L.NE.1 .OR. I.EQ.1) GO TO 70
      WRITE(IOUT,8)
    8 FORMAT(1H0,'AQUIFER TYPE 1 IS ONLY ALLOWED IN TOP LAYER')
      STOP
C
C3C3----LAYER TYPES 1 AND 3 NEED A BOTTOM. ADD 1 TO KB.
   70 IF(L.EQ.1 .OR. L.EQ.3) NBOT=NBOT+1
C
C3C4----LAYER TYPES 2 AND 3 NEED A TOP. ADD 1 TO KT.
      IF(L.EQ.2 .OR. L.EQ.3) NTOP=NTOP+1
  100 CONTINUE
C
C
C
C4------COMPUTE DIMENSIONS FOR ARRAYS.
      NRC=NROW*NCOL
      ISIZ=NRC*NLAY
C
C5------ALLOCATE SPACE FOR ARRAYS. IF RUN IS TRANSIENT(ISS=0)
C5------THEN SPACE MUST BE ALLOCATED FOR STORAGE.
      ISOLD=ISUM
      LCSC1=ISUM
      IF(ISS.EQ.0) ISUM=ISUM+ISIZ
      LCSC2=ISUM
      IF(ISS.EQ.0) ISUM=ISUM+NRC*NTOP
      LCTRPY=ISUM
      ISUM=ISUM+NLAY
      LCBOT=ISUM
      ISUM=ISUM+NRC*NBOT
      LCHY=ISUM
      ISUM=ISUM+NRC*NBOT
      LCTOP=ISUM
      ISUM=ISUM+NRC*NTOP
C
C6------PRINT THE AMOUNT OF SPACE USED BY THE BCF PACKAGE.
      ISP=ISUM-ISOLD
      WRITE(IOUT,101) ISP
  101 FORMAT(1X,I8,' ELEMENTS IN X ARRAY ARE USED BY BCF')
      ISUM1=ISUM-1
      WRITE(IOUT,102) ISUM1,LENX
  102 FORMAT(1X,I8,' ELEMENTS OF X ARRAY USED OUT OF',I8)
      IF(ISUM1.GT.LENX) WRITE(IOUT,103)
  103 FORMAT(1X,'   ***X ARRAY MUST BE DIMENSIONED LARGER***')
C
C7------RETURN
      RETURN
      END
```

```
      SUBROUTINE BCF1RP(IBOUND,HNEW,SC1,HY,CR,CC,CV,DELR,DELC,
     1          BOT,TOP,SC2,TRPY,IN,ISS,NCOL,NROW,NLAY,NODES,IOUT)
C
C-----VERSION 1636 15MAY1987 BCF1RP
C
C     ******************************************************************
C     READ AND INITIALIZE DATA FOR BLOCK-CENTERED FLOW PACKAGE
C     ******************************************************************
C
C     SPECIFICATIONS:
C     ------------------------------------------------------------------
      CHARACTER*4 ANAME
      DOUBLE PRECISION HNEW
C
      DIMENSION HNEW(NODES),SC1(NODES),HY(NODES),CR(NODES),CC(NODES),
     1          CV(NODES),ANAME(6,10),DELR(NCOL),DELC(NROW),BOT(NODES),
     1          TOP(NODES),SC2(NODES),TRPY(NLAY),IBOUND(NODES)
C
      COMMON /FLWCOM/LAYCON(80)
C
      DATA ANAME(1,1),ANAME(2,1),ANAME(3,1),ANAME(4,1),ANAME(5,1),
     1 ANAME(6,1) /'    ','PRIM','ARY ','STOR','AGE ','COEF'/
      DATA ANAME(1,2),ANAME(2,2),ANAME(3,2),ANAME(4,2),ANAME(5,2),
     1 ANAME(6,2) /'    ','TRAN','SMIS','. AL','ONG ','ROWS'/
      DATA ANAME(1,3),ANAME(2,3),ANAME(3,3),ANAME(4,3),ANAME(5,3),
     1 ANAME(6,3) /'   H','YD. ','COND','. AL','ONG ','ROWS'/
      DATA ANAME(1,4),ANAME(2,4),ANAME(3,4),ANAME(4,4),ANAME(5,4),
     1 ANAME(6,4) /'VERT',' HYD',' CON','D /T','HICK','NESS'/
      DATA ANAME(1,5),ANAME(2,5),ANAME(3,5),ANAME(4,5),ANAME(5,5),
     1 ANAME(6,5) /'    ','    ','    ','    ','  BO','TTOM'/
      DATA ANAME(1,6),ANAME(2,6),ANAME(3,6),ANAME(4,6),ANAME(5,6),
     1 ANAME(6,6) /'    ','    ','    ','    ','    ',' TOP'/
      DATA ANAME(1,7),ANAME(2,7),ANAME(3,7),ANAME(4,7),ANAME(5,7),
     1 ANAME(6,7) /' SE','COND','ARY ','STOR','AGE ','COEF'/
      DATA ANAME(1,8),ANAME(2,8),ANAME(3,8),ANAME(4,8),ANAME(5,8),
     1 ANAME(6,8) /'COLU','MN T','O RO','W AN','ISOT','ROPY'/
      DATA ANAME(1,9),ANAME(2,9),ANAME(3,9),ANAME(4,9),ANAME(5,9),
     1 ANAME(6,9) /'    ','    ','    ','    ','    ','DELR'/
      DATA ANAME(1,10),ANAME(2,10),ANAME(3,10),ANAME(4,10),ANAME(5,10),
     1 ANAME(6,10) /'    ','    ','    ','    ','    ','DELC'/
C     ------------------------------------------------------------------
C
C1------CALCULATE NUMBER OF NODES IN A LAYER AND READ TRPY,DELR,DELC
      NIJ=NCOL*NROW
C
      CALL U1DREL(TRPY,ANAME(1,8),NLAY,IN,IOUT)
      CALL U1DREL(DELR,ANAME(1,9),NCOL,IN,IOUT)
      CALL U1DREL(DELC,ANAME(1,10),NROW,IN,IOUT)
```

```
C
C2------READ ALL PARAMETERS FOR EACH LAYER
      KT=0
      KB=0
      DO 200 K=1,NLAY
      KK=K
C
C2A-----FIND ADDRESS OF EACH LAYER IN THREE DIMENSION ARRAYS.
      IF(LAYCON(K).EQ.1 .OR. LAYCON(K).EQ.3) KB=KB+1
      IF(LAYCON(K).EQ.2 .OR. LAYCON(K).EQ.3) KT=KT+1
      LOC=1+(K-1)*NIJ
      LOCB=1+(KB-1)*NIJ
      LOCT=1+(KT-1)*NIJ
C
C2B-----READ PRIMARY STORAGE COEFFICIENT INTO ARRAY SC1 IF TRANSIENT
      IF(ISS.EQ.0)CALL U2DREL(SC1(LOC),ANAME(1,1),NROW,NCOL,KK,IN,IOUT)
C
C2C-----READ TRANSMISSIVITY INTO ARRAY CC IF LAYER TYPE IS 0 OR 2
      IF(LAYCON(K).EQ.3 .OR. LAYCON(K).EQ.1) GO TO 100
      CALL U2DREL(CC(LOC),ANAME(1,2),NROW,NCOL,KK,IN,IOUT)
      GO TO 110
C
C2D-----READ HYDRAULIC CONDUCTIVITY(HY) AND BOTTOM ELEVATION(BOT)
C2D-----IF LAYER TYPE IS 1 OR 3
  100 CALL U2DREL(HY(LOCB),ANAME(1,3),NROW,NCOL,KK,IN,IOUT)
      CALL U2DREL(BOT(LOCB),ANAME(1,5),NROW,NCOL,KK,IN,IOUT)
C
C2E-----READ VERTICAL HYCOND/THICK INTO ARRAY CV IF NOT BOTTOM LAYER
C2E----- READ AS HYCOND/THICKNESS -- CONVERTED TO CONDUCTANCE LATER
  110 IF(K.EQ.NLAY) GO TO 120
      CALL U2DREL(CV(LOC),ANAME(1,4),NROW,NCOL,KK,IN,IOUT)
C
C2F-----READ SECONDARY STORAGE COEFFICIENT INTO ARRAY SC2 IF TRANSIENT
C2F-----AND LAYER TYPE IS 2 OR 3
  120 IF(LAYCON(K).NE.3 .AND. LAYCON(K).NE.2) GO TO 200
      IF(ISS.EQ.0)CALL U2DREL(SC2(LOCT),ANAME(1,7),NROW,NCOL,KK,IN,IOUT)
C
C2G-----READ TOP ELEVATION(TOP) IF LAYER TYPE IS 2 OR 3
      CALL U2DREL(TOP(LOCT),ANAME(1,6),NROW,NCOL,KK,IN,IOUT)
  200 CONTINUE
C
C3------PREPARE AND CHECK BCF DATA
      CALL SBCF1N(HNEW,IBOUND,SC1,SC2,CR,CC,CV,HY,TRPY,DELR,DELC,ISS,
     1            NCOL,NROW,NLAY,IOUT)
C
C4------RETURN
      RETURN
      END
```

```
          SUBROUTINE BCF1FM(HCOF,RHS,HOLD,SC1,HNEW,IBOUND,CR,CC,CV,HY,TRPY,
         1               BOT,TOP,SC2,DELR,DELC,DELT,ISS,KITER,KSTP,KPER,
         2               NCOL,NROW,NLAY,IOUT)
C-----VERSION 1640 15MAY1987 BCF1FM
C
C     ****************************************************************
C     ADD LEAKAGE CORRECTION AND STORAGE TO HCOF AND RHS, AND CALCULATE
C     CONDUCTANCE AS REQUIRED
C     ****************************************************************
C
C        SPECIFICATIONS:
C     ----------------------------------------------------------------
      DOUBLE PRECISION HNEW
C
      DIMENSION HCOF(NCOL,NROW,NLAY),RHS(NCOL,NROW,NLAY),
     1    HOLD(NCOL,NROW,NLAY),SC1(NCOL,NROW,NLAY),HNEW(NCOL,NROW,NLAY),
     2    IBOUND(NCOL,NROW,NLAY),CR(NCOL,NROW,NLAY),
     3    CC(NCOL,NROW,NLAY),CV(NCOL,NROW,NLAY),HY(NCOL,NROW,NLAY),
     4    TRPY(NLAY),BOT(NCOL,NROW,NLAY),TOP(NCOL,NROW,NLAY),DELR(NCOL),
     5    DELC(NROW),SC2(NCOL,NROW,NLAY)
C
      COMMON /FLWCOM/LAYCON(80)
C     ----------------------------------------------------------------
      KB=0
      KT=0
C
C1------FOR EACH LAYER: IF T VARIES CALCULATE HORIZONTAL CONDUCTANCES
      DO 100 K=1,NLAY
      KK=K
      IF(LAYCON(K).EQ.3 .OR. LAYCON(K).EQ.2) KT=KT+1
C
C1A-----IF LAYER TYPE IS NOT 1 OR 3 THEN SKIP THIS LAYER.
      IF(LAYCON(K).NE.3 .AND. LAYCON(K).NE.1) GO TO 100
      KB=KB+1
C
C1B-----FOR LAYER TYPES 1 & 3 CALL SBCFH1 TO CALCULATE
C1B-----HORIZONTAL CONDUCTANCES.
      CALL SBCF1H(HNEW,IBOUND,CR,CC,CV,HY,TRPY,DELR,DELC,BOT,TOP,
     1           KK,KB,KT,KITER,KSTP,KPER,NCOL,NROW,NLAY,IOUT)
  100 CONTINUE
C
C2------IF THE SIMULATION IS TRANSIENT ADD STORAGE TO HCOF AND RHS
      IF(ISS.NE.0) GO TO 201
      TLED=1./DELT
      KT=0
      DO 200 K=1,NLAY
C
C3------SEE IF THIS LAYER IS CONVERTIBLE OR NON-CONVERTIBLE.
      IF(LAYCON(K).EQ.3 .OR. LAYCON(K).EQ.2) GO TO 150
C4------NON-CONVERTIBLE LAYER, SO USE PRIMARY STORAGE
      DO 140 I=1,NROW
      DO 140 J=1,NCOL
      IF(IBOUND(J,I,K).LE.0) GO TO 140
      RHO=SC1(J,I,K)*TLED
      HCOF(J,I,K)=HCOF(J,I,K)-RHO
      RHS(J,I,K)=RHS(J,I,K)-RHO*HOLD(J,I,K)
  140 CONTINUE
      GO TO 200
C
C5------A CONVERTIBLE LAYER, SO CHECK OLD AND NEW HEADS TO DETERMINE
C5------WHEN TO USE PRIMARY AND SECONDARY STORAGE
  150 KT=KT+1
      DO 180 I=1,NROW
      DO 180 J=1,NCOL
C
C5A-----IF THE CELL IS EXTERNAL THEN SKIP IT.
      IF(IBOUND(J,I,K).LE.0) GO TO 180
      TP=TOP(J,I,KT)
      RHO2=SC2(J,I,KT)*TLED
```

```
                 RHO1=SC1(J,I,K)*TLED
      C
      CSB-----FIND STORAGE FACTOR AT START OF TIME STEP.
                 SOLD=RHO2
                 IF(HOLD(J,I,K).GT.TP) SOLD=RHO1
      C
      CSC-----FIND STORAGE FACTOR AT END OF TIME STEP.
                 HTMP=HNEW(J,I,K)
                 SNEW=RHO2
                 IF(HTMP.GT.TP) SNEW=RHO1
      C
      C5D-----ADD STORAGE TERMS TO RHS AND HCOF.
                 HCOF(J,I,K)=HCOF(J,I,K)-SNEW
                 RHS(J,I,K)=RHS(J,I,K) - SOLD*(HOLD(J,I,K)-TP) - SNEW*TP
      C
         180 CONTINUE
      C
         200 CONTINUE
      C
      C6------FOR EACH LAYER DETERMINE IF CORRECTION TERMS ARE NEEDED FOR
      C6------FLOW DOWN INTO PARTIALLY SATURATED LAYERS.
         201 KT=0
                 DO 300 K=1,NLAY
      C
      C7------SEE IF CORRECTION IS NEEDED FOR LEAKAGE FROM ABOVE.
                 IF(LAYCON(K).NE.3 .AND. LAYCON(K).NE.2) GO TO 250
                 KT=KT+1
                 IF(K.EQ.1) GO TO 250
      C
      C7A-----FOR EACH CELL MAKE THE CORRECTION IF NEEDED.
                 DO 220 I=1,NROW
                 DO 220 J=1,NCOL
      C
      C7B-----IF THE CELL IS EXTERNAL(IBOUND<=0) THEN SKIP IT.
                 IF(IBOUND(J,I,K).LE.0) GO TO 220
                 HTMP=HNEW(J,I,K)
      C
      C7C-----IF HEAD IS ABOVE TOP THEN CORRECTION NOT NEEDED
                 IF(HTMP.GE.TOP(J,I,KT)) GO TO 220
      C
      C7D-----WITH HEAD BELOW TOP ADD CORRECTION TERMS TO RHS AND HCOF.
                 RHS(J,I,K)=RHS(J,I,K) + CV(J,I,K-1)*TOP(J,I,KT)
                 HCOF(J,I,K)=HCOF(J,I,K) + CV(J,I,K-1)
         220 CONTINUE
      C
      C8------SEE IF THIS LAYER MAY NEED CORRECTION FOR LEAKAGE TO BELOW.
         250 IF(K.EQ.NLAY) GO TO 300
                 IF(LAYCON(K+1).NE.3 .AND. LAYCON(K+1).NE.2) GO TO 300
                 KTT=KT+1
      C
      C8A-----FOR EACH CELL MAKE THE CORRECTION IF NEEDED.
                 DO 280 I=1,NROW
                 DO 280 J=1,NCOL
      C
      C8B-----IF CELL IS EXTERNAL (IBOUND<=0) THEN SKIP IT.
                 IF(IBOUND(J,I,K).LE.0) GO TO 280
      C
      C8C-----IF HEAD IN THE LOWER CELL IS LESS THAN TOP ADD CORRECTION
      C8C-----TERM TO RHS.
                 HTMP=HNEW(J,I,K+1)
                 IF(HTMP.LT.TOP(J,I,KTT)) RHS(J,I,K)=RHS(J,I,K)
             1                          - CV(J,I,K)*(TOP(J,I,KTT)-HTMP)
         280 CONTINUE
         300 CONTINUE
      C
      C9------RETURN
                 RETURN
                 END
```

```
              SUBROUTINE BCF1BD(VBNM,VBVL,MSUM,HNEW,IBOUND,HOLD,SC1,CR,CC,CV,
            1    TOP,SC2,DELT,ISS,NCOL,NROW,NLAY,KSTP,KPER,IBCFCB,
            2    ICBCFL,BUFF,IOUT)
C-----VERSION 1546 12MAY1987 BCF1BD
C
C     ******************************************************************
C     COMPUTE BUDGET FLOW TERMS FOR BCF -- STORAGE, CONSTANT HEAD, AND
C     FLOW ACROSS CELL WALLS
C     ******************************************************************
C
C     SPECIFICATIONS:
C     ------------------------------------------------------------------
      CHARACTER*4 VBNM,TEXT
      DOUBLE PRECISION HNEW
C
      DIMENSION HNEW(NCOL,NROW,NLAY), IBOUND(NCOL,NROW,NLAY),
     1    .HOLD(NCOL,NROW,NLAY), SC1(NCOL,NROW,NLAY),
     2    CR(NCOL,NROW,NLAY), CC(NCOL,NROW,NLAY),
     3    CV(NCOL,NROW,NLAY), VBNM(4,20), VBVL(4,20),
     4    SC2(NCOL,NROW,NLAY),
     5    TOP(NCOL,NROW,NLAY),BUFF(NCOL,NROW,NLAY)
C
      COMMON /FLWCOM/LAYCON(80)
C
      DIMENSION TEXT(4)
C
      DATA TEXT(1),TEXT(2),TEXT(3),TEXT(4) /'    ','    ',' STO','RAGE'/
C     ------------------------------------------------------------------
C
C1------INITIALIZE BUDGET ACCUMULATORS
      STOIN=0.
      STOUT=0.
C
C2------IF CELL-BY-CELL FLOWS ARE NEEDED THEN SET FLAG IBD.
      IBD=0
      IF(ICBCFL.NE.0 .AND. IBCFCB.GT.0) IBD=1
C
C3------IF STEADY STATE THEN SKIP ALL STORAGE CALCULATIONS
      IF(ISS.NE.0) GO TO 305
C
C4------IF CELL-BY-CELL FLOWS ARE NEEDED (IBD IS SET) CLEAR BUFFER
      IF(IBD.EQ.0) GO TO 220
      DO 210 K=1,NLAY
      DO 210 I=1,NROW
      DO 210 J=1,NCOL
      BUFF(J,I,K)=0.
  210 CONTINUE
C
C5------RUN THROUGH EVERY CELL IN THE GRID
  220 KT=0
      DO 300 K=1,NLAY
      LC=LAYCON(K)
      IF(LC.EQ.3 .OR. LC.EQ.2) KT=KT+1
      DO 300 I=1,NROW
      DO 300 J=1,NCOL
C
C6------CALCULATE FLOW FROM STORAGE (VARIABLE HEAD CELLS ONLY)
```

```
      IF(IBOUND(J,I,K).LE.0) GO TO 300
      HSING=HNEW(J,I,K)
C
C6A----CHECK LAYER TYPE TO SEE IF ONE STORAGE CAPACITY OR TWO
      IF(LC.NE.3 .AND. LC.NE.2) GO TO 285
C
C6B----TWO STORAGE CAPACITIES
      TP=TOP(J,I,KT)
      SYA=SC2(J,I,KT)
      SCFA=SC1(J,I,K)
      SOLD=SYA
      IF(HOLD(J,I,K).GT.TP) SOLD=SCFA
      SNEW=SYA
      IF(HSING.GT.TP) SNEW=SCFA
      STRG=SOLD*(HOLD(J,I,K)-TP) + SNEW*TP - SNEW*HSING
      GO TO 288
C
C6C----ONE STORAGE CAPACITY
  285 SC=SC1(J,I,K)
      STRG=SC*HOLD(J,I,K) - SC*HSING
C
C7-----STORE CELL-BY-CELL FLOW IN BUFFER AND ADD TO ACCUMULATORS
  288 IF(IBD.EQ.1) BUFF(J,I,K)=STRG/DELT
      IF(STRG) 292,300,294
  292 STOUT=STOUT-STRG
      GO TO 300
  294 STOIN=STOIN+STRG
C
  300 CONTINUE
C
C8-----IF IBD FLAG IS SET RECORD THE CONTENTS OF THE BUFFER
      IF(IBD.EQ.1) CALL UBUDSV(KSTP,KPER,TEXT,
     1                         IBCFCB,BUFF,NCOL,NROW,NLAY,IOUT)
C
C9------ADD TOTAL RATES AND VOLUMES TO VBVL & PUT TITLES IN VBNM
  305 VBVL(1,MSUM)=VBVL(1,MSUM)+STOIN
      VBVL(2,MSUM)=VBVL(2,MSUM)+STOUT
      VBVL(3,MSUM)=STOIN/DELT
      VBVL(4,MSUM)=STOUT/DELT
      VBNM(1,MSUM)=TEXT(1)
      VBNM(2,MSUM)=TEXT(2)
      VBNM(3,MSUM)=TEXT(3)
      VBNM(4,MSUM)=TEXT(4)
      MSUM=MSUM+1
C
C10-----CALCULATE FLOW FROM CONSTANT HEAD NODES
      CALL SBCF1F(VBNM,VBVL,MSUM,HNEW,IBOUND,CR,CC,CV,TOP,DELT,
     1       NCOL,NROW,NLAY,KSTP,KPER,IBD,IBCFCB,ICBCFL,BUFF,IOUT)
C
C11-----CALCULATE AND SAVE FLOW ACROSS CELL BOUNDARIES IF C-B-C
C11-----FLOW TERMS ARE REQUESTED.
      IF(IBD.NE.0) CALL SBCF1B(HNEW,IBOUND,CR,CC,CV,TOP,NCOL,NROW,NLAY,
     1       KSTP,KPER,IBCFCB,BUFF,IOUT)
C
C12----RETURN
      RETURN
      END
```

```
      SUBROUTINE SBCF1N(HNEW,IBOUND,SC1,SC2,CR,CC,CV,HY,TRPY,DELR,DELC,
     1           ISS,NCOL,NROW,NLAY,IOUT)
C
C-----VERSION 1642 15MAY1987 SBCF1N
C
C     ****************************************************************
C     INITIALIZE AND CHECK BCF DATA
C     ****************************************************************
C
C        SPECIFICATIONS:
C     ----------------------------------------------------------------
C
      DOUBLE PRECISION HNEW,HCNV
C
      DIMENSION HNEW(NCOL,NROW,NLAY),IBOUND(NCOL,NROW,NLAY)
     1     ,SC1(NCOL,NROW,NLAY),CR(NCOL,NROW,NLAY)
     2     ,CC(NCOL,NROW,NLAY),CV(NCOL,NROW,NLAY)
     3     ,HY(NCOL,NROW,NLAY),TRPY(NLAY),DELR(NCOL),DELC(NROW)
     4     ,SC2(NCOL,NROW,NLAY)
C
      COMMON /FLWCOM/LAYCON(80)
C     ----------------------------------------------------------------
C
C1------IF IBOUND=0, SET CV=0., CC=0., AND HY=0.
      KB=0
      DO 30 K=1,NLAY
      IF(LAYCON(K).EQ.3 .OR. LAYCON(K).EQ.1) KB=KB+1
      DO 30 I=1,NROW
      DO 30 J=1,NCOL
      IF(IBOUND(J,I,K).NE.0) GO TO 30
      IF(K.NE.NLAY) CV(J,I,K)=0.
      IF(K.NE.1) CV(J,I,K-1)=0.
      CC(J,I,K)=0.
      IF(LAYCON(K).EQ.3 .OR. LAYCON(K).EQ.1) HY(J,I,KB)=0.
   30 CONTINUE
C
C2------INSURE THAT EACH ACTIVE CELL HAS AT LEAST ONE NON-ZERO
C2------TRANSMISSIVE PARAMETER. IF NOT, CONVERT CELL TO NOFLOW.
      HCNV=888.88
      KB=0
      DO 60 K=1,NLAY
      IF(LAYCON(K).EQ.1 .OR. LAYCON(K).EQ.3) GO TO 55
C2A-----WHEN LAYER TYPE 0 OR 2, TRANSMISSIVITY OR CV MUST BE NONZERO
      DO 54 I=1,NROW
      DO 54 J=1,NCOL
      IF(IBOUND(J,I,K).EQ.0) GO TO 54
      IF(CC(J,I,K).NE.0.) GO TO 54
      IF(K.EQ.NLAY) GO TO 51
      IF(CV(J,I,K).NE.0.) GO TO 54
   51 IF(K.EQ.1) GO TO 53
      IF(CV(J,I,K-1).NE.0.) GO TO 54
   53 IBOUND(J,I,K)=0
      HNEW(J,I,K)=HCNV
      WRITE(IOUT,52) K,I,J
   52 FORMAT(1X,'NODE (LAYER,ROW,COL)',3I4,
     1     ' ELIMINATED BECAUSE ALL CONDUCTANCES TO NODE ARE 0')
   54 CONTINUE
      GO TO 60
```

```
C
C2B-----WHEN LAYER TYPE IS 1 OR 3, HY OR CV MUST BE NONZERO
   55 KB=KB+1
      DO 59 I=1,NROW
      DO 59 J=1,NCOL
      IF(IBOUND(J,I,K).EQ.0) GO TO 59
      IF(HY(J,I,KB).NE.0.) GO TO 59
      IF(K.EQ.NLAY) GO TO 56
      IF(CV(J,I,K).NE.0.) GO TO 59
   56 IF(K.EQ.1) GO TO 57
      IF(CV(J,I,K-1).NE.0.) GO TO 59
   57 IBOUND(J,I,K)=0
      HNEW(J,I,K)=HCNV
      CC(J,I,K)=0.
      WRITE(IOUT,52) K,I,J
   59 CONTINUE
   60 CONTINUE
C
C3------CALCULATE HOR. CONDUCTANCE(CR AND CC) FOR CONSTANT T LAYERS
      DO 65 K=1,NLAY
      KK=K
      IF(LAYCON(K).EQ.3 .OR. LAYCON(K).EQ.1) GO TO 65
      CALL SBCF1C(CR,CC,TRPY,DELR,DELC,KK,NCOL,NROW,NLAY)
   65 CONTINUE
C
C4------MULTIPLY VERTICAL LEAKANCE BY AREA TO MAKE CONDUCTANCE
      IF(NLAY.EQ.1) GO TO 69
      K1=NLAY-1
      DO 68 K=1,K1
      DO 68 I=1,NROW
      DO 68 J=1,NCOL
      CV(J,I,K)=CV(J,I,K)*DELR(J)*DELC(I)
   68 CONTINUE
C
C5------IF TRANSIENT MULTIPLY PRIMARY STORAGE COEFFICIENT BY DELR &
C5------DELC TO GET PRIMARY STORAGE CAPACITY(SC1).
   69 IF(ISS.NE.0) GO TO 100
      KT=0
      DO 80 K=1,NLAY
      DO 70 I=1,NROW
      DO 70 J=1,NCOL
      SC1(J,I,K)=SC1(J,I,K)*DELR(J)*DELC(I)
   70 CONTINUE
C
C6------IF LAYER IS CONF/UNCONF MULTIPLY SECONDARY STORAGE COEFFICIENT
C6------BY DELR AND DELC TO GET SECONDARY STORAGE CAPACITY(SC2).
      IF(LAYCON(K).NE.3 .AND. LAYCON(K).NE.2) GO TO 80
      KT=KT+1
      DO 75 I=1,NROW
      DO 75 J=1,NCOL
      SC2(J,I,KT)=SC2(J,I,KT)*DELR(J)*DELC(I)
   75 CONTINUE
C
   80 CONTINUE
C
C7------RETURN
  100 RETURN
      END
```

```
      SUBROUTINE SBCF1C(CR,CC,TRPY,DELR,DELC,K,NCOL,NROW,NLAY)
C
C
C-----VERSION 1334 22AUG1987 SBCF1C
C     ********************************************************************
C     COMPUTE BRANCH CONDUCTANCE USING HARMONIC MEAN OF BLOCK
C     CONDUCTANCES -- BLOCK TRANSMISSIVITY IS IN CC UPON ENTRY
C     ********************************************************************
C
C     SPECIFICATIONS:
C     ------------------------------------------------------------------
C
      DIMENSION CR(NCOL,NROW,NLAY), CC(NCOL,NROW,NLAY)
     2    , TRPY(NLAY), DELR(NCOL), DELC(NROW)
C
C     ------------------------------------------------------------------
      YX=TRPY(K)*2.
C
C1------FOR EACH CELL CALCULATE BRANCH CONDUCTANCES FROM THAT CELL
C1------TO THE ONE ON THE RIGHT AND THE ONE IN FRONT.
      DO 40 I=1,NROW
      DO 40 J=1,NCOL
      T1=CC(J,I,K)
C
C2------IF T=0 THEN SET CONDUCTANCE EQUAL TO 0. GO ON TO NEXT CELL.
      IF(T1.NE.0.) GO TO 10
      CR(J,I,K)=0.
      GO TO 40
C
C3------IF THIS IS NOT THE LAST COLUMN(RIGHTMOST) THEN CALCULATE
C3------BRANCH CONDUCTANCE IN THE ROW DIRECTION (CR) TO THE RIGHT.
   10 IF(J.EQ.NCOL) GO TO 30
      T2=CC(J+1,I,K)
      CR(J,I,K)=2.*T2*T1*DELC(I)/(T1*DELR(J+1)+T2*DELR(J))
C
C4------IF THIS IS NOT THE LAST ROW(FRONTMOST) THEN CALCULATE
C4------BRANCH CONDUCTANCE IN THE COLUMN DIRECTION (CC) TO THE FRONT.
   30 IF(I.EQ.NROW) GO TO 40
      T2=CC(J,I+1,K)
      CC(J,I,K)=YX*T2*T1*DELR(J)/(T1*DELC(I+1)+T2*DELC(I))
   40 CONTINUE
C
C5------RETURN
      RETURN
      END
```

```
      SUBROUTINE SBCF1B(HNEW,IBOUND,CR,CC,CV,TOP,NCOL,NROW,NLAY,
     1        KSTP,KPER,IBCFCB,BUFF,IOUT)
C
C-----VERSION 1548 12MAY1987 SBCF1B
C
C     ******************************************************************
C     COMPUTE FLOW ACROSS EACH CELL WALL
C     ******************************************************************
C
C     SPECIFICATIONS:
C     ------------------------------------------------------------------
      CHARACTER*4 TEXT
      DOUBLE PRECISION HNEW,HD
C
      DIMENSION HNEW(NCOL,NROW,NLAY), IBOUND(NCOL,NROW,NLAY),
     1      CR(NCOL,NROW,NLAY), CC(NCOL,NROW,NLAY),
     2      CV(NCOL,NROW,NLAY), TOP(NCOL,NROW,NLAY),
     3      BUFF(NCOL,NROW,NLAY)
C
      COMMON /FLWCOM/LAYCON(80)
C
      DIMENSION TEXT(12)
C
      DATA TEXT(1),TEXT(2),TEXT(3),TEXT(4),TEXT(5),TEXT(6),TEXT(7),
     1    TEXT(8),TEXT(9),TEXT(10),TEXT(11),TEXT(12)
     2    /'FLOW',' RIG','HT F','ACE ',
     2     'FLOW',' FRO','NT F','ACE ','FLOW',' LOW','ER F','ACE '/
C     ------------------------------------------------------------------
C
      NCM1=NCOL-1
      IF(NCM1.LT.1) GO TO 405
C
C1-----CLEAR THE BUFFER
      DO 310 K=1,NLAY
      DO 310 I=1,NROW
      DO 310 J=1,NCOL
      BUFF(J,I,K)=0.
  310 CONTINUE
C
C2-----FOR EACH CELL CALCULATE FLOW THRU RIGHT FACE & STORE IN BUFFER
      DO 400 K=1,NLAY
      DO 400 I=1,NROW
      DO 400 J=1,NCM1
      IF((IBOUND(J,I,K).LE.0) .AND. (IBOUND(J+1,I,K).LE.0)) GO TO 400
      HDIFF=HNEW(J,I,K)-HNEW(J+1,I,K)
      BUFF(J,I,K)=HDIFF*CR(J,I,K)
  400 CONTINUE
C
C3-----RECORD CONTENTS OF BUFFER
      CALL UBUDSV(KSTP,KPER,TEXT(1),IBCFCB,BUFF,NCOL,NROW,NLAY,IOUT)
C
```

```
C4-----CLEAR THE BUFFER
   405 NRM1=NROW-1
       IF(NRM1.LT.1) GO TO 505
       DO 410 K=1,NLAY
       DO 410 I=1,NROW
       DO 410 J=1,NCOL
       BUFF(J,I,K)=0.
   410 CONTINUE
C
C5-----FOR EACH CELL CALCULATE FLOW THRU FRONT FACE & STORE IN BUFFER
       DO 500 K=1,NLAY
       DO 500 I=1,NRM1
       DO 500 J=1,NCOL
       IF((IBOUND(J,I,K).LE.0) .AND. (IBOUND(J,I+1,K).LE.0)) GO TO 500
       HDIFF=HNEW(J,I,K)-HNEW(J,I+1,K)
       BUFF(J,I,K)=HDIFF*CC(J,I,K)
   500 CONTINUE
C
C6-----RECORD CONTENTS OF BUFFER.
       CALL UBUDSV(KSTP,KPER,TEXT(5),IBCFCB,BUFF,NCOL,NROW,NLAY,IOUT)
   505 NLM1=NLAY-1
       IF(NLM1.LT.1) GO TO 1000
C
C7-----CLEAR THE BUFFER
       DO 510 K=1,NLAY
       DO 510 I=1,NROW
       DO 510 J=1,NCOL
       BUFF(J,I,K)=0.
   510 CONTINUE
C
C8-----FOR EACH CELL CALCULATE FLOW THRU LOWER FACE & STORE IN BUFFER
       KT=0
       DO 600 K=1,NLM1
       IF(LAYCON(K).EQ.3 .OR. LAYCON(K).EQ.2) KT=KT+1
       DO 600 I=1,NROW
       DO 600 J=1,NCOL
       IF((IBOUND(J,I,K).LE.0) .AND. (IBOUND(J,I,K+1).LE.0)) GO TO 600
       HD=HNEW(J,I,K+1)
       IF(LAYCON(K+1).NE.3 .AND. LAYCON(K+1).NE.2) GO TO 580
       TMP=HD
       IF(TMP.LT.TOP(J,I,KT+1)) HD=TOP(J,I,KT+1)
   580 HDIFF=HNEW(J,I,K)-HD
       BUFF(J,I,K)=HDIFF*CV(J,I,K)
   600 CONTINUE
C
C9-----RECORD CONTENTS OF BUFFER.
       CALL UBUDSV(KSTP,KPER,TEXT(9),IBCFCB,BUFF,NCOL,NROW,NLAY,IOUT)
C
C10----RETURN
  1000 RETURN
       END
```

```
      SUBROUTINE SBCF1F(VBNM,VBVL,MSUM,HNEW,IBOUND,CR,CC,CV,
     1    TOP,DELT,NCOL,NROW,NLAY,KSTP,KPER,IBD,IBCFCB,ICBCFL,
     2    BUFF,IOUT)
C-----VERSION 1549 12MAY1987 SBCF1F
C
C     ******************************************************************
C     COMPUTE FLOW FROM CONSTANT HEAD NODES
C     ******************************************************************
C
C     SPECIFICATIONS:
C     ------------------------------------------------------------------
      CHARACTER*4 VBNM,TEXT
      DOUBLE PRECISION HNEW,HD
C
      DIMENSION HNEW(NCOL,NROW,NLAY), IBOUND(NCOL,NROW,NLAY),
     1    CR(NCOL,NROW,NLAY), CC(NCOL,NROW,NLAY),
     2    CV(NCOL,NROW,NLAY), VBNM(4,20), VBVL(4,20),
     3    TOP(NCOL,NROW,NLAY),BUFF(NCOL,NROW,NLAY)
C
      COMMON /FLWCOM/LAYCON(80)
C
      DIMENSION TEXT(4)
C
      DATA TEXT(1),TEXT(2),TEXT(3),TEXT(4) /'   C','ONST','ANT ','HEAD'/
C     ------------------------------------------------------------------
C
C1------CLEAR BUDGET ACCUMULATORS
      CHIN=0.
      CHOUT=0.
C
C2------CLEAR BUFFER IF CELL-BY-CELL FLOW TERM FLAG(IBD) IS SET
      IF(IBD.EQ.0) GO TO 8
      DO 5 K=1,NLAY
      DO 5 I=1,NROW
      DO 5 J=1,NCOL
      BUFF(J,I,K)=0.
    5 CONTINUE
C
C3------FOR EACH CELL IF IT IS CONSTANT HEAD COMPUTE FLOW ACROSS 6
C3------FACES.
    8 KT=0
      DO 200 K=1,NLAY
      LC=LAYCON(K)
      IF(LC.EQ.3 .OR. LC.EQ.2) KT=KT+1
      DO 200 I=1,NROW
      DO 200 J=1,NCOL
C
C4------IF CELL IS NOT CONSTANT HEAD SKIP IT & GO ON TO NEXT CELL.
      IF (IBOUND(J,I,K).GE.0)GO TO 200
C
C5------CLEAR FIELDS FOR SIX FLOW RATES.
      X1=0.
      X2=0.
      X3=0.
      X4=0.
      X5=0.
      X6=0.
C6------FOR EACH FACE OF THE CELL CALCULATE FLOW THROUGH THAT FACE
C6------OUT OF THE CONSTANT HEAD CELL AND INTO THE FLOW DOMAIN.
C6------COMMENTS 7-11 APPEAR ONLY IN THE SECTION HEADED BY COMMENT 6A
C6------BUT THEY APPLY IN A SIMILAR MANNER TO THE SECTIONS HEADED
C6------BY COMMENTS 6B-6F.
C
```

```
C6A----CALCULATE FLOW THROUGH THE LEFT FACE
C
C7-----IF THERE IS NOT A VARIABLE HEAD CELL ON THE OTHER SIDE OF THIS
C7-----FACE THEN GO ON TO THE NEXT FACE.
      IF(J.EQ.1) GO TO 30
      IF(IBOUND(J-1,I,K).LE.0)GO TO 30
      HDIFF=HNEW(J,I,K)-HNEW(J-1,I,K)
C
C8-----CALCULATE FLOW THROUGH THIS FACE INTO THE ADJACENT CELL.
      X1=HDIFF*CR(J-1,I,K)
C
C9-----TEST TO SEE IF FLOW IS POSITIVE OR NEGATIVE
      IF (X1) 10,30,20
C
C10----IF NEGATIVE ADD TO CHOUT(FLOW OUT OF DOMAIN TO CONSTANT HEAD).
   10 CHOUT=CHOUT-X1
      GO TO 30
C
C11----IF POSITIVE ADD TO CHIN(FLOW INTO DOMAIN FROM CONSTANT HEAD).
   20 CHIN=CHIN+X1
C
C6B----CALCULATE FLOW THROUGH THE RIGHT FACE
   30 IF(J.EQ.NCOL) GO TO 60
      IF(IBOUND(J+1,I,K).LE.0) GO TO 60
      HDIFF=HNEW(J,I,K)-HNEW(J+1,I,K)
      X2=HDIFF*CR(J,I,K)
      IF(X2)40,60,50
   40 CHOUT=CHOUT-X2
      GO TO 60
   50 CHIN=CHIN+X2
C
C6C----CALCULATE FLOW THROUGH THE BACK FACE.
   60 IF(I.EQ.1) GO TO 90
      IF (IBOUND(J,I-1,K).LE.0) GO TO 90
      HDIFF=HNEW(J,I,K)-HNEW(J,I-1,K)
      X3=HDIFF*CC(J,I-1,K)
      IF(X3) 70,90,80
   70 CHOUT=CHOUT-X3
      GO TO 90
   80 CHIN=CHIN+X3
C
C6D----CALCULATE FLOW THROUGH THE FRONT FACE.
   90 IF(I.EQ.NROW) GO TO 120
      IF(IBOUND(J,I+1,K).LE.0) GO TO 120
      HDIFF=HNEW(J,I,K)-HNEW(J,I+1,K)
      X4=HDIFF*CC(J,I,K)
      IF (X4) 100,120,110
  100 CHOUT=CHOUT-X4
      GO TO 120
  110 CHIN=CHIN+X4
C
C6E----CALCULATE FLOW THROUGH THE UPPER FACE
  120 IF(K.EQ.1) GO TO 150
      IF (IBOUND(J,I,K-1).LE.0) GO TO 150
      HD=HNEW(J,I,K)
      IF(LC.NE.3 .AND. LC.NE.2) GO TO 122
      TMP=HD
      IF(TMP.LT.TOP(J,I,KT)) HD=TOP(J,I,KT)
  122 HDIFF=HD-HNEW(J,I,K-1)
      X5=HDIFF*CV(J,I,K-1)
      IF(X5) 130,150,140
  130 CHOUT=CHOUT-X5
      GO TO 150
  140 CHIN=CHIN+X5
```

```
C
C6F----CALCULATE FLOW THROUGH THE LOWER FACE.
  150 IF(K.EQ.NLAY) GO TO 180
      IF(IBOUND(J,I,K+1).LE.0) GO TO 180
      HD=HNEW(J,I,K+1)
      IF(LAYCON(K+1).NE.3 .AND. LAYCON(K+1).NE.2) GO TO 152
      TMP=HD
      IF(TMP.LT.TOP(J,I,KT+1)) HD=TOP(J,I,KT+1)
  152 HDIFF=HNEW(J,I,K)-HD
      X6=HDIFF*CV(J,I,K)
      IF(X6) 160,180,170
  160 CHOUT=CHOUT-X6
      GO TO 180
  170 CHIN=CHIN+X6
C
C12-----SUM UP FLOWS THROUGH SIX SIDES OF CONSTANT HEAD CELL.
  180  RATE=X1+X2+X3+X4+X5+X6
C
C13-----PRINT THE INDIVIDUAL RATES IF REQUESTED(IBCFCB<0).
      IF(IBCFCB.LT.0.AND.ICBCFL.NE.0) WRITE(IOUT,900) (TEXT(N),N=1,4),
     1    KPER,KSTP,K,I,J,RATE
  900 FORMAT(1H0,4A4,'   PERIOD',I3,'   STEP',I3,'   LAYER',I3,
     1    '   ROW',I4,'   COL',I4,'   RATE ',G15.7)
C
C14----IF CELL-BY-CELL FLAG SET STORE SUM OF FLOWS FOR CELL IN BUFFER
      IF(IBD.EQ.1) BUFF(J,I,K)=RATE
C
  200 CONTINUE
C
C15----IF CELL-BY-CELL FLAG SET THEN RECORD CONTENTS OF BUFFER
      IF(IBD.EQ.1) CALL UBUDSV(KSTP,KPER,TEXT(1),
     1                    IBCFCB,BUFF,NCOL,NROW,NLAY,IOUT)
C
C
C16----SAVE TOTAL CONSTANT HEAD FLOWS AND VOLUMES IN VBVL TABLE
C16----FOR INCLUSION IN BUDGET. PUT LABELS IN VBNM TABLE.
      VBVL(1,MSUM)=VBVL(1,MSUM)+CHIN*DELT
      VBVL(2,MSUM)=VBVL(2,MSUM)+CHOUT*DELT
      VBVL(3,MSUM)=CHIN
      VBVL(4,MSUM)=CHOUT
C
C     ---SETUP VOLUMETRIC BUDGET NAMES
      VBNM(1,MSUM)=TEXT(1)
      VBNM(2,MSUM)=TEXT(2)
      VBNM(3,MSUM)=TEXT(3)
      VBNM(4,MSUM)=TEXT(4)
C
      MSUM=MSUM+1
C
C
C17----RETURN
      RETURN
      END
```

Module Documentation for the Strongly Implicit Procedure Package

The Stongly Implicit Procedure Package (SIP1) consists of three primary
modules and two submodules. They are:

Primary Modules

SIP1AL   Allocates space for SIP work arrays.

SIP1RP   Reads control information needed by the SIP
          Package and calculates iteration parameters if
          the seed is specified by the user.

SIP1AP   Performs one iteration of the strongly implicit
          procedure.

Submodules

SSIP1P   Prints the largest head change for each iteration.

SSIP1I   Calculates iteration parameters when the seed
          is calculated by the program.

```fortran
      SUBROUTINE SIP1AL(ISUM,LENX,LCEL,LCFL,LCGL,LCV,LCHDCG,LCLRCH,
     1          LCW,MXITER,NPARM,NCOL,NROW,NLAY,IN,IOUT)
C
C-----VERSION 1110 31DEC1986 SIP1AL
C
C     ********************************************************************
C     ALLOCATE STORAGE IN THE X ARRAY FOR SIP ARRAYS
C     ********************************************************************
C
C        SPECIFICATIONS:
C     ------------------------------------------------------------------
C     ------------------------------------------------------------------
C
C1------PRINT A MESSAGE IDENTIFYING SIP PACKAGE
      WRITE(IOUT,1)IN
    1 FORMAT(1H0,'SIP1 -- STRONGLY IMPLICIT PROCEDURE SOLUTION PACKAGE'
     1,', VERSION 1, 9/1/87',' INPUT READ FROM UNIT',I3)
C
C2------READ AND PRINT MXITER AND NPARM
      READ(IN,2) MXITER,NPARM
    2 FORMAT(2I10)
      WRITE(IOUT,3) MXITER,NPARM
    3 FORMAT(1X,'MAXIMUM OF',I4,' ITERATIONS ALLOWED FOR CLOSURE'/
     1      1X,I2,' ITERATION PARAMETERS')
C
C3------ALLOCATE SPACE FOR THE SIP ARRAYS
      ISOLD=ISUM
      NRC=NROW*NCOL
      ISIZ=NRC*NLAY
      LCEL=ISUM
      ISUM=ISUM+ISIZ
      LCFL=ISUM
      ISUM=ISUM+ISIZ
      LCGL=ISUM
      ISUM=ISUM+ISIZ
      LCV=ISUM
      ISUM=ISUM+ISIZ
      LCHDCG=ISUM
      ISUM=ISUM+MXITER
      LCLRCH=ISUM
      ISUM=ISUM+3*MXITER
      LCW=ISUM
      ISUM=ISUM+NPARM
C
C4------CALCULATE AND PRINT THE SPACE USED IN THE X ARRAY
      ISP=ISUM-ISOLD
      WRITE(IOUT,4) ISP
    4 FORMAT(1X,I8,' ELEMENTS IN X ARRAY ARE USED BY SIP')
      ISUM1=ISUM-1
      WRITE(IOUT,5) ISUM1,LENX
    5 FORMAT(1X,I8,' ELEMENTS OF X ARRAY USED OUT OF',I8)
      IF(ISUM1.GT.LENX) WRITE(IOUT,6)
    6 FORMAT(1X,'   ***X ARRAY MUST BE DIMENSIONED LARGER***')
C
C5------RETURN
      RETURN
      END
```

```
      SUBROUTINE SIP1RP(NPARM,MXITER,ACCL,HCLOSE,W,IN,IPCALC,IPRSIP,
     1                  IOUT)
C
C-----VERSION 0925 16DEC1982 SIP1RP
C
C     ******************************************************************
C     READ DATA FOR SIP
C     ******************************************************************
C
C        SPECIFICATIONS:
C     ------------------------------------------------------------------
      DIMENSION W(NPARM)
C     ------------------------------------------------------------------
C
C1------READ ACCL,HCLOSE,WSEED,IPCALC,IPRSIP
      READ(IN,1) ACCL,HCLOSE,IPCALC,WSEED,IPRSIP
    1 FORMAT(2F10.0,I10,F10.0,I10)
      IF(ACCL.EQ.0.) ACCL=1.
C
C2------PRINT DATA VALUES JUST READ
      WRITE(IOUT,100)
  100 FORMAT(1H0,///57X,'SOLUTION BY THE STRONGLY IMPLICIT PROCEDURE'
     1/57X,43('-'))
      WRITE(IOUT,115) MXITER
  115 FORMAT(1H0,47X,'MAXIMUM ITERATIONS ALLOWED FOR CLOSURE =',I9)
      WRITE(IOUT,120) ACCL
  120 FORMAT(1H ,63X,'ACCELERATION PARAMETER =',G15.5)
      WRITE(IOUT,125) HCLOSE
  125 FORMAT(1H ,52X,'HEAD CHANGE CRITERION FOR CLOSURE =',E15.5)
      IF(IPRSIP.LE.0)IPRSIP=999
      WRITE(IOUT,130) IPRSIP
  130 FORMAT(1H ,52X,'SIP HEAD CHANGE PRINTOUT INTERVAL =',I9)
C
C3------CHECK IF SPECIFIED VALUE OF WSEED SHOULD BE USED OR IF
C3------SEED SHOULD BE CALCULATED
      IF(IPCALC.EQ.0) GO TO 150
C
C3A-----CALCULATE SEED & ITERATION PARAMETERS PRIOR TO 1ST ITERATION
      WRITE(IOUT,140)
  140 FORMAT(1H0,52X,'CALCULATE ITERATION PARAMETERS FROM MODEL',
     1' CALCULATED WSEED')
      GO TO 1000
C
C3B-----USE SPECIFIED VALUE OF WSEED
C3B-----CALCULATE AND PRINT ITERATION PARAMETERS
  150 P1=-1.
      P2=NPARM-1
      DO 160 I=1,NPARM
      P1=P1+1.
  160 W(I)=1.-WSEED**(P1/P2)
      WRITE(IOUT,161) NPARM,WSEED,(W(J),J=1,NPARM)
  161 FORMAT(1H0,/,I5,' ITERATION PARAMETERS CALCULATED FROM',
     1       ' SPECIFIED WSEED =',F11.8,' :'//(10X,6E15.7))
C
C4------RETURN
 1000 RETURN
      END
```

```
          SUBROUTINE SIP1AP(HNEW,IBOUND,CR,CC,CV,HCOF,RHS,EL,FL,GL,V,
        1       W,HDCG,LRCH,NPARM,KITER,HCLOSE,ACCL,ICNVG,KSTP,KPER,
        2       IPCALC,IPRSIP,MXITER,NSTP,NCOL,NROW,NLAY,NODES,IOUT)
C-----VERSION 1656 24JUL1987 SIP1AP
C
C     ******************************************************************
C     SOLUTION BY THE STRONGLY IMPLICIT PROCEDURE -- 1 ITERATION
C     ******************************************************************
C
C        SPECIFICATIONS:
C     ------------------------------------------------------------------
      DOUBLE PRECISION HNEW,DITPAR,AC,HHCOF,RRHS,XI,DZERO,DONE,RES
      DOUBLE PRECISION Z,B,D,E,F,H,S,AP,TP,CP,GP,UP,RP
      DOUBLE PRECISION ZHNEW,BHNEW,DHNEW,FHNEW,HHNEW,SHNEW
      DOUBLE PRECISION AL,BL,CL,DL,ELNCL,FLNCL,GLNCL
      DOUBLE PRECISION ELNRL,FLNRL,GLNRL,ELNLL,FLNLL,GLNLL
      DOUBLE PRECISION VNRL,VNCL,VNLL,ELXI,FLXI,GLXI,VN,HCFHNW
C
      DIMENSION HNEW(NODES),IBOUND(NODES),CR(NODES),CC(NODES),
        1 CV(NODES),HCOF(NODES),RHS(NODES),EL(NODES),FL(NODES),
        2 GL(NODES),V(NODES),W(NPARM),HDCG(MXITER),LRCH(3,MXITER)
C     ------------------------------------------------------------------
C
C1------CALCULATE ITERATION PARAMETERS IF FLAG IS SET.  THEN
C1------CLEAR THE FLAG SO THAT CALCULATION IS DONE ONLY ONCE.
      IF(IPCALC.NE.0)
        1     CALL SSIP1I(CR,CC,CV,IBOUND,NPARM,W,NCOL,NROW,NLAY,IOUT)
      IPCALC=0
C
C2------ASSIGN VALUES TO FIELDS THAT ARE CONSTANT DURING AN ITERATION
      DZERO=0.
      DONE=1.
      AC=ACCL
      NRC=NROW*NCOL
      NTH=MOD(KITER-1,NPARM)+1
      DITPAR=W(NTH)
C
C3------INITIALIZE VARIABLE THAT TRACKS MAXIMUM HEAD CHANGE DURING
C3------THE ITERATION
      BIGG=0.
C
C4------CLEAR SIP WORK ARRAYS.
      DO 100 I=1,NODES
      EL(I)=0.
      FL(I)=0.
      GL(I)=0.
  100 V(I)=0.
C
C5------SET NORMAL/REVERSE EQUATION ORDERING FLAG (1 OR -1) AND
C5------CALCULATE INDEXES DEPENDENT ON ORDERING
      IDIR=1
      IF(MOD(KITER,2).EQ.0)IDIR=-1
      IDNRC=IDIR*NRC
      IDNCOL=IDIR*NCOL
C
C6------STEP THROUGH CELLS CALCULATING INTERMEDIATE VECTOR V
C6------USING FORWARD SUBSTITUTION
      DO 150 K=1,NLAY
      DO 150 I=1,NROW
      DO 150 J=1,NCOL
C
C6A-----SET UP CURRENT CELL LOCATION INDEXES.  THESE ARE DEPENDENT
C6A-----ON THE DIRECTION OF EQUATION ORDERING.
      IF(IDIR.LE.0)GO TO 120
      II=I
      JJ=J
      KK=K
      GO TO 122
  120 II=NROW-I+1
      JJ=J
      KK=NLAY-K+1
```

```
C
C6B-----CALCULATE 1 DIMENSIONAL SUBSCRIPT OF CURRENT CELL AND
C6B-----SKIP CALCULATIONS IF CELL IS NOFLOW OR CONSTANT HEAD
   122 N=JJ+(II-1)*NCOL+(KK-1)*NRC
       IF(IBOUND(N).LE.0)GO TO 150
C
C6C-----CALCULATE 1 DIMENSIONAL SUBSCRIPTS FOR LOCATING THE 6
C6C-----SURROUNDING CELLS
       NRN=N+IDNCOL
       NRL=N-IDNCOL
       NCN=N+1
       NCL=N-1
       NLN=N+IDNRC
       NLL=N-IDNRC
C
C6D-----CALCULATE 1 DIMENSIONAL SUBSCRIPTS FOR CONDUCTANCE TO THE 6
C6D-----SURROUNDING CELLS.  THESE DEPEND ON ORDERING OF EQUATIONS.
       IF(IDIR.LE.0)GO TO 124
       NCF=N
       NCD=NCL
       NRB=NRL
       NRH=N
       NLS=N
       NLZ=NLL
       GO TO 126
   124 NCF=N
       NCD=NCL
       NRB=N
       NRH=NRN
       NLS=NLN
       NLZ=N
C
C6E------ASSIGN VARIABLES IN MATRICES A & U INVOLVING ADJACENT CELLS
C6E1----NEIGHBOR IS 1 ROW BACK
   126 B=DZERO
       ELNRL=DZERO
       FLNRL=DZERO
       GLNRL=DZERO
       BHNEW=DZERO
       VNRL=DZERO
       IF(I.EQ.1) GO TO 128
       B=CC(NRB)
       ELNRL=EL(NRL)
       FLNRL=FL(NRL)
       GLNRL=GL(NRL)
       BHNEW=B*HNEW(NRL)
       VNRL=V(NRL)
C
C6E2----NEIGHBOR IS 1 ROW AHEAD
   128 H=DZERO
       HHNEW=DZERO
       IF(I.EQ.NROW) GO TO 130
       H=CC(NRH)
       HHNEW=H*HNEW(NRN)
C
C6E3----NEIGHBOR IS 1 COLUMN BACK
   130 D=DZERO
       ELNCL=DZERO
       FLNCL=DZERO
       GLNCL=DZERO
       DHNEW=DZERO
       VNCL=DZERO
       IF(J.EQ.1) GO TO 132
       D=CR(NCD)
       ELNCL=EL(NCL)
       FLNCL=FL(NCL)
       GLNCL=GL(NCL)
       DHNEW=D*HNEW(NCL)
       VNCL=V(NCL)
```

```
C
C6E4----NEIGHBOR IS 1 COLUMN AHEAD
   132 F=DZERO
       FHNEW=DZERO
       IF(J.EQ.NCOL) GO TO 134
       F=CR(NCF)
       FHNEW=F*HNEW(NCN)
C
C6E5----NEIGHBOR IS 1 LAYER BEHIND
   134 Z=DZERO
       ELNLL=DZERO
       FLNLL=DZERO
       GLNLL=DZERO
       ZHNEW=DZERO
       VNLL=DZERO
       IF(K.EQ.1) GO TO 136
       Z=CV(NLZ)
       ELNLL=EL(NLL)
       FLNLL=FL(NLL)
       GLNLL=GL(NLL)
       ZHNEW=Z*HNEW(NLL)
       VNLL=V(NLL)
C
C6E6----NEIGHBOR IS 1 LAYER AHEAD
   136 S=DZERO
       SHNEW=DZERO
       IF(K.EQ.NLAY) GO TO 138
       S=CV(NLS)
       SHNEW=S*HNEW(NLN)
C
C6E7----CALCULATE THE NEGATIVE SUM OF ALL CONDUCTANCES TO NEIGHBORING
C6E7----CELLS
   138 E=-Z-B-D-F-H-S
C
C6F-----CALCULATE COMPONENTS OF THE UPPER AND LOWER MATRICES, WHICH
C6F-----ARE THE FACTORS OF MATRIX (A+B)
       AL=Z/(DONE+DITPAR*(ELNLL+FLNLL))
       BL=B/(DONE+DITPAR*(ELNRL+GLNRL))
       CL=D/(DONE+DITPAR*(FLNCL+GLNCL))
       AP=AL*ELNLL
       CP=BL*ELNRL
       GP=CL*FLNCL
       RP=CL*GLNCL
       TP=AL*FLNLL
       UP=BL*GLNRL
       HHCOF=HCOF(N)
       DL=E+HHCOF+DITPAR*(AP+TP+CP+GP+UP+RP)-AL*GLNLL-BL*FLNRL-CL*ELNCL
       EL(N)=(F-DITPAR*(AP+CP))/DL
       FL(N)=(H-DITPAR*(TP+GP))/DL
       GL(N)=(S-DITPAR*(RP+UP))/DL
C
C6G-----CALCULATE THE RESIDUAL
       RRHS=RHS(N)
       HNW=HNEW(N)
       HCFHNW=HNW*HCOF(N)
       RES=RRHS-ZHNEW-BHNEW-DHNEW-E*HNEW(N)-HCFHNW-FHNEW-HHNEW-SHNEW
C
C6H-----CALCULATE THE INTERMEDIATE VECTOR V
       V(N)=(AC*RES-AL*VNLL-BL*VNRL-CL*VNCL)/DL
C
   150 CONTINUE
C
C7------STEP THROUGH EACH CELL AND SOLVE FOR HEAD CHANGE BY BACK
C7------SUBSTITUTION
       DO 160 K=1,NLAY
       DO 160 I=1,NROW
       DO 160 J=1,NCOL
C
```

```
C7A-----SET UP CURRENT CELL LOCATION INDEXES.  THESE ARE DEPENDENT
C7A-----ON THE DIRECTION OF EQUATION ORDERING.
      IF(IDIR.LT.0) GO TO 152
      KK=NLAY-K+1
      II=NROW-I+1
      JJ=NCOL-J+1
      GO TO 154
  152 KK=K
      II=I
      JJ=NCOL-J+1
C
C7B-----CALCULATE 1 DIMENSIONAL SUBSCRIPT OF CURRENT CELL AND
C7B-----SKIP CALCULATIONS IF CELL IS NOFLOW OR CONSTANT HEAD
  154 N=JJ+(II-1)*NCOL+(KK-1)*NRC
      IF(IBOUND(N).LE.0)GO TO 160
C
C7C-----CALCULATE 1 DIMENSIONAL SUBSCRIPTS FOR THE 3 NEIGHBORING CELLS
C7C-----BEHIND (RELATIVE TO THE DIRECTION OF THE BACK SUBSTITUTION
C7C-----ORDERING) THE CURRRENT CELL.
      NC=N+1
      NR=N+IDNCOL
      NL=N+IDNRC
C
C7D-----BACK SUBSTITUTE, STORING HEAD CHANGE IN ARRAY V IN PLACE OF
C7D-----INTERMEDIATE FORWARD SUBSTITUTION VALUES.
      ELXI=DZERO
      FLXI=DZERO
      GLXI=DZERO
      IF(JJ.NE.NCOL) ELXI=EL(N)*V(NC)
      IF(I.NE.I) FLXI=FL(N)*V(NR)
      IF(K.NE.1) GLXI=GL(N)*V(NL)
      VN=V(N)
      V(N)=VN-ELXI-FLXI-GLXI
C
C7E-----GET THE ABSOLUTE HEAD CHANGE. IF IT IS MAX OVER GRID SO FAR.
C7E-----THEN SAVE IT ALONG WITH CELL INDICES AND HEAD CHANGE.
      TCHK=ABS(V(N))
      IF (TCHK.LE.BIGG) GO TO 155
      BIGG=TCHK
      BIG=V(N)
      IB=II
      JB=JJ
      KB=KK
C
C7F-----ADD HEAD CHANGE THIS ITERATION TO HEAD FROM THE PREVIOUS
C7F-----ITERATION TO GET A NEW ESTIMATE OF HEAD.
  155 XI=V(N)
      HNEW(N)=HNEW(N)+XI
C
  160 CONTINUE
C
C8------STORE THE LARGEST ABSOLUTE HEAD CHANGE (THIS ITERATION) AND
C8------AND ITS LOCATION.
      HDCG(KITER)=BIG
      LRCH(1,KITER)=KB
      LRCH(2,KITER)=IB
      LRCH(3,KITER)=JB
      ICNVG=0
      IF(BIGG.LE.HCLOSE) ICNVG=1
C
C9------IF END OF TIME STEP, PRINT # OF ITERATIONS THIS STEP
      IF(ICNVG.EQ.0 .AND. KITER.NE.MXITER) GO TO 600
      IF(KSTP.EQ.1) WRITE(IOUT,500)
  500 FORMAT(1H0)
      WRITE(IOUT,501) KITER,KSTP,KPER
  501 FORMAT(1X,I5,' ITERATIONS FOR TIME STEP',I4,' IN STRESS PERIOD',
     1      I3)
C
C10-----PRINT HEAD CHANGE EACH ITERATION IF PRINTOUT INTERVAL IS REACHED
      IF(ICNVG.EQ.0 .OR. KSTP.EQ.NSTP .OR. MOD(KSTP,IPRSIP).EQ.0)
     1      CALL SSIP1P(HDCG,LRCH,KITER,MXITER,IOUT)
C
C11-----RETURN
  600   RETURN
C
      END
```

```fortran
      SUBROUTINE SSIP1P(HDCG,LRCH,KITER,MXITER,IOUT)
C
C
C-----VERSION 1636 24JUL1987 SSIP1P
C     ******************************************************************
C     PRINT MAXIMUM HEAD CHANGE FOR EACH ITERATION DURING A TIME STEP
C     ******************************************************************
C
C        SPECIFICATIONS:
C     ------------------------------------------------------------------
C
      DIMENSION HDCG(MXITER), LRCH(3,MXITER)
C     ------------------------------------------------------------------
C
      WRITE(IOUT,5)
    5 FORMAT(1H0,'MAXIMUM HEAD CHANGE FOR EACH ITERATION:'/
     1    1H0,5(' HEAD CHANGE LAYER,ROW,COL')/1X,132('-'))
      WRITE (IOUT,10) (HDCG(J),(LRCH(I,J),I=1,3),J=1,KITER)
   10 FORMAT((1X,5(G12.4,' (',I3,',',I3,',',I3,')')))
      WRITE(IOUT,11)
   11 FORMAT(1H0)
C
      RETURN
C
      END
```

```
      SUBROUTINE SSIP1I(CR,CC,CV,IBOUND,NPARM,W,NCOL,NROW,NLAY,
     1            IOUT)
C
C-----VERSION 1417 12MAY1987 SSIP1I
C     ******************************************************************
C     CALCULATE AN ITERATION PARAMETER SEED AND USE IT TO CALCULATE SIP
C     ITERATION PARAMETERS
C     ******************************************************************
C
C        SPECIFICATIONS:
C     ------------------------------------------------------------------
      DIMENSION CR(NCOL,NROW,NLAY),CC(NCOL,NROW,NLAY)
     1          ,CV(NCOL,NROW,NLAY),IBOUND(NCOL,NROW,NLAY),W(NPARM)
C
      DOUBLE PRECISION DWMIN,AVGSUM
C     ------------------------------------------------------------------
C
C1------CALCULATE CONSTANTS AND INITIALIZE VARIABLES
      PIEPIE=9.869604
      R=NROW
      C=NCOL
      ZL=NLAY
      CCOL=PIEPIE/(2.*C*C)
      CROW=PIEPIE/(2.*R*R)
      CLAY=PIEPIE/(2.*ZL*ZL)
      WMINMN=1.
      AVGSUM=0.
      NODES=0
C
C2------LOOP THROUGH ALL CELLS, CALCULATING A SEED FOR EACH CELL
C2------THAT IS ACTIVE
      DO 100 K=1,NLAY
      DO 100 I=1,NROW
      DO 100 J=1,NCOL
      IF(IBOUND(J,I,K).LE.0) GO TO 100
C
C2A-----CONDUCTANCE FROM THIS CELL
C2A-----TO EACH OF THE 6 ADJACENT CELLS
      D=0.
      IF(J.NE.1) D=CR(J-1,I,K)
      F=0.
      IF(J.NE.NCOL) F=CR(J,I,K)
      B=0.
      IF(I.NE.1) B=CC(J,I-1,K)
      H=0.
      IF(I.NE.NROW) H=CC(J,I,K)
      Z=0.
      IF(K.NE.1) Z=CV(J,I,K-1)
      S=0.
      IF(K.NE.NLAY) S=CV(J,I,K)
C
C2B-----FIND THE MAXIMUM AND MINIMUM OF THE 2 CONDUCTANCE COEFFICIENTS
C2B-----IN EACH PRINCIPAL COORDINATE DIRECTION
```

```
      DFMX=AMAX1(D,F)
      BHMX=AMAX1(B,H)
      ZSMX=AMAX1(Z,S)
      DFMN=AMIN1(D,F)
      BHMN=AMIN1(B,H)
      ZSMN=AMIN1(Z,S)
      IF(DFMN.EQ.0.) DFMN=DFMX
      IF(BHMN.EQ.0.) BHMN=BHMX
      IF(ZSMN.EQ.0.) ZSMN=ZSMX
C
C2C-----CALCULATE A SEED IN EACH PRINCIPAL COORDINATE DIRECTION
      WCOL=1.
      IF(DFMN.NE.0.) WCOL=CCOL/(1.+(BHMX+ZSMX)/DFMN)
      WROW=1.
      IF(BHMN.NE.0.) WROW=CROW/(1.+(DFMX+ZSMX)/BHMN)
      WLAY=1.
      IF(ZSMN.NE.0.) WLAY=CLAY/(1.+(DFMX+BHMX)/ZSMN)
C
C2D-----SELECT THE CELL SEED, WHICH IS THE MINIMUM SEED OF THE 3.
C2D-----SELECT THE MINIMUM SEED OVER THE WHOLE GRID.
      WMIN=AMIN1(WCOL,WROW,WLAY)
      WMINMN=AMIN1(WMINMN,WMIN)
C
C2E-----ADD THE CELL SEED TO THE ACCUMULATOR AVGSUM FOR USE
C2E-----IN GETTING THE AVERAGE SEED.
      DWMIN=WMIN
      AVGSUM=AVGSUM+DWMIN
      NODES=NODES+1
C
  100 CONTINUE
C
C3------CALCULATE THE AVERAGE SEED OF THE CELL SEEDS, AND PRINT
C3------THE AVERAGE AND MINIMUM SEEDS.
      TMP=NODES
      AVGMIN=AVGSUM
      AVGMIN=AVGMIN/TMP
      WRITE(IOUT,101) AVGMIN,WMINMN
  101 FORMAT(1H0,'AVERAGE SEED =',F11.8/1X,'MINIMUM SEED =',F11.8)
C
C4------CALCULATE AND PRINT ITERATION PARAMETERS FROM THE AVERAGE SEED
      P1=-1.
      P2=NPARM-1
      DO 50 I=1,NPARM
      P1=P1+1.
   50 W(I)=1.-AVGMIN**(P1/P2)
      WRITE(IOUT,150) NPARM,(W(J),J=1,NPARM)
  150 FORMAT(1H0,/,I5,' ITERATION PARAMETERS CALCULATED FROM',
     1        ' AVERAGE SEED:'//(10X,6E15.7))
C
C5------RETURN
      RETURN
      END
```

APPENDIX A.2

MT3D DOCUMENTATION

Hydro-Search, Inc.

M T 3 D

a modular three-dimensional transport model

User's Manual
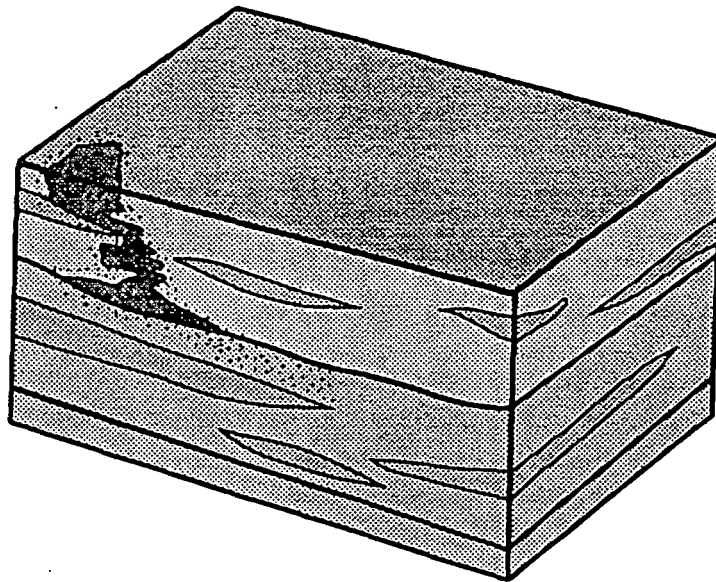
PREFACE

This document describes the theory and application of MT3D: a modular three-dimensional transport model for simulation of advection, dispersion and chemical reactions in groundwater systems. It includes four computer disks containing the MT3D source code, example data sets, post-processing programs, and a flow model to be used in conjunction with MT3D. A supplemental document which contains a complete listing of the MT3D source code is available if there is a need to verify the source code included in the computer disk.

The documentation for the MT3D program has been funded in part by the United States Environmental Protection Agency. However, the funding does not constitute endorsement or recommendation by the United States Environmental Protection Agency for the use of MT3D or any commercial products mentioned in the document.

To report any error in the MT3D program or to inquire about future upgrades, please call or write to

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S.S. Papadopulos & Associates, Inc.

Table of Contents

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 a modular structure similar to that implemented in MODFLOW, the U. S. Geological Survey 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 for 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.

The 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 will 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 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.

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 computer 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 a 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. Geological Survey modular three-dimensional finite-difference groundwater flow model, referred to as MODFLOW, (McDonald and Harbaugh, 1988). The modular structure of the transport model 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 modify 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 the 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 used 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 explicit 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 a 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 requirements of the MT3D model and its interface with a flow model; printout of sample input and output files; explanation of several post-processing programs and tables of abbreviated input instructions.

1.4 ACKNOWLEDGEMENTS

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_i 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};

θ 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):

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

where

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

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

λ is the rate constant of the first-order rate reactions, T^{-1}.

By rewriting the $\dfrac{\rho_b}{\theta}\dfrac{\partial \bar{C}}{\partial t}$ term as:

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

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

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

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

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

where R is called the retardation factor, defined as

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

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:

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

(2.8)

where S_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), $\frac{\partial}{\partial x_i}(v_iC)$, 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:

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

(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. 2.1a). The second type of numerical problem is artificial oscillation, sometimes also referred to as overshoot and undershoot, as illustrated in Fig. 2.1b. 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 ∞ 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 region than 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

(a) Effect of numerical dispersion

— Analytical —◆— Numerical

(b) Effect of artificial oscillation

— Analytical —◆— Numerical
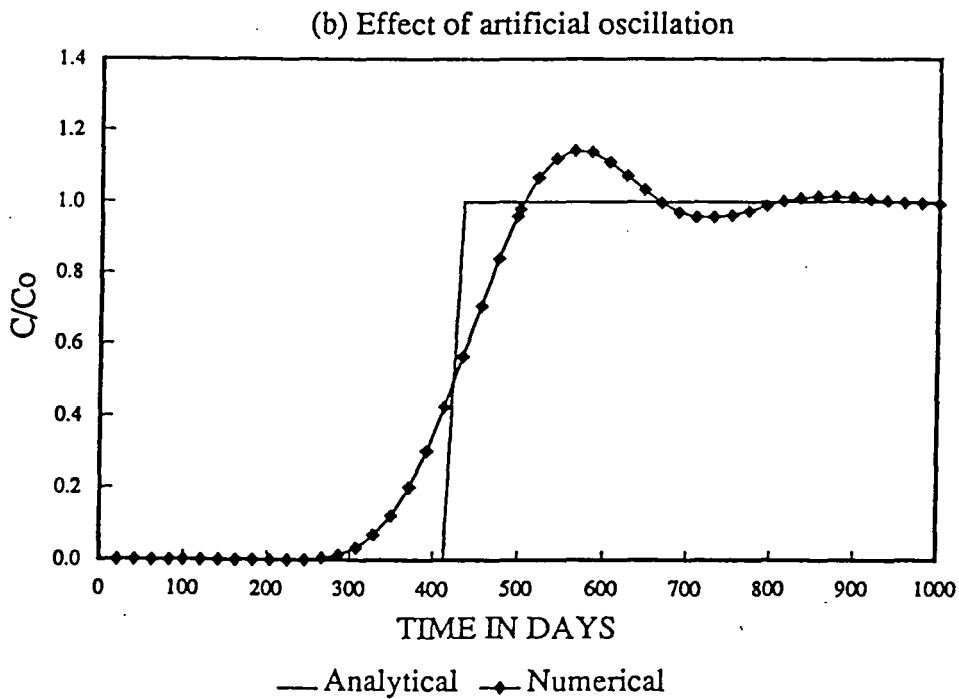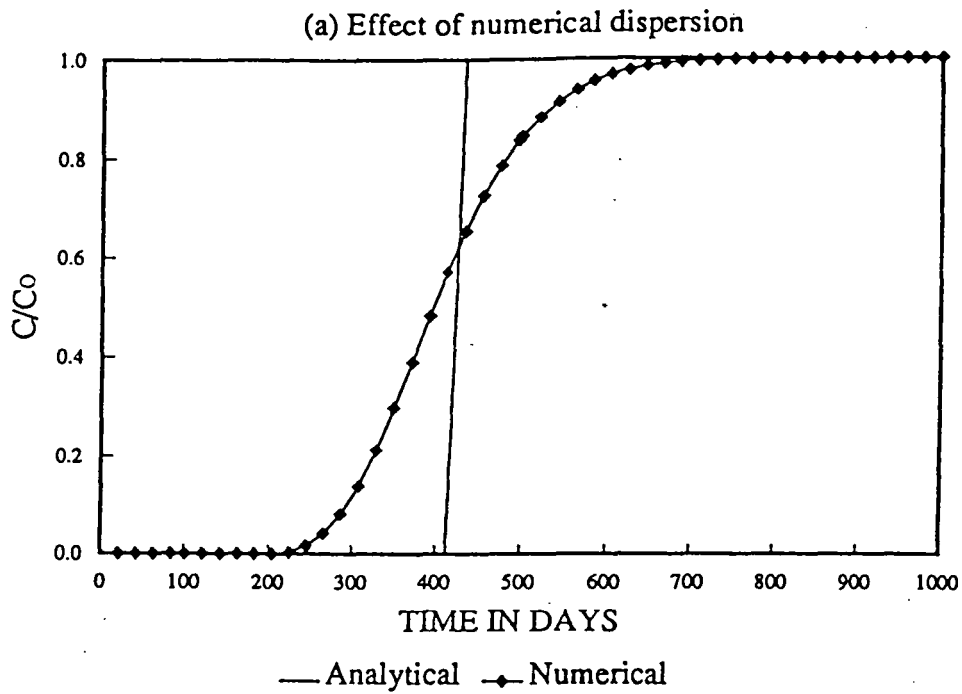
Fig. 2.1. Illustration of common numerical errors in contaminant transport modeling.

groundwater velocity is very low. The sum of the mechanical dispersion and the molecular diffusion is termed hydrodynamic dispersion.

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), $\dfrac{\partial}{\partial x_i}\left(D_{ij}\dfrac{\partial C}{\partial x_j}\right)$, 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:

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

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

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

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

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

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

where

α_L is the longitudinal dispersivity, L;

α_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};

$|v| = \left(v_x^2 + v_y^2 + v_z^2 \right)^{1/2}$ 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 (α_{TH}) and a vertical transverse dispersivity (α_{TV}), as proposed by Burnett and Frind (1987):

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

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

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

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

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

$$D_{yz} = D_{zy} = \left(\alpha_L - \alpha_{TV} \right) \frac{v_y v_z}{|v|} \tag{2.10f}$$

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 aquifer 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 ($\bar{C}$) is directly proportional to the dissolved concentration (C):

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

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

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

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

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

where

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

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:

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

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

$$\bar{C} = \frac{K_l \bar{S} C}{1 + K_l C}$$

(2.15)

where

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

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

The retardation factor defined for the Langmuir isotherm is then

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

(2.16)

2.5.2 Radioactive Decay or Biodegradation

The first-order irreversible rate reaction term included in the governing equation,

$-\lambda \left(C + \frac{\rho_b}{\theta} \bar{C} \right)$, represents the mass loss of both the dissolved phase (C) and the sorbed phase

($\bar{C}$) with the same rate constant rate (λ). The rate constant is usually given in terms of the half-life:

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

(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 (λ_1) and the other for the sorbed phase (λ_2) as shown below:

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

(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

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

where

$C^\circ(x,y,z)$ is a known concentration distribution and $\forall$ 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,

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

where Γ_1 denotes the specified-concentration boundary, and $C^\circ(x,y,z)$ is the specified concentration along Γ_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 simulated 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,

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

where $q(x,y,z,t)$ is a known function representing the dispersive flux normal to the boundary Γ_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,

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

where $g(x,y,z,t)$ is a known function representing the total flux (dispersive and advective) normal to the boundary Γ_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

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

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

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

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

Equation (3.2) is an Eulerian expression in which the partial derivative, $\frac{\partial C}{\partial t}$, 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

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

where the substantial derivative, $\frac{DC}{Dt} = \frac{\partial C}{\partial t} + \bar{v}_i \frac{\partial C}{\partial x_i}$, 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

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

(3.4)

so that equation (3.3) becomes

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

(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 $(n+1)$ due to advection alone, also referred to as the intermediate time level (n^*);

Δt is the time increment between the old time level (n) and the new time level $(n+1)$;

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. This is expressed in the following equation (also see Fig. 3.1):

$$C_m^{n*} = \frac{1}{NP} \sum_{l=1}^{NP} C_l^n$$

(3.6)

where

NP is the number of particles within cell m;

C_l^n is the concentration of the lth 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 :

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

(3.7)

MOC

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

$$\frac{1}{NP}\sum_{l=1}^{NP} C_l^n$$
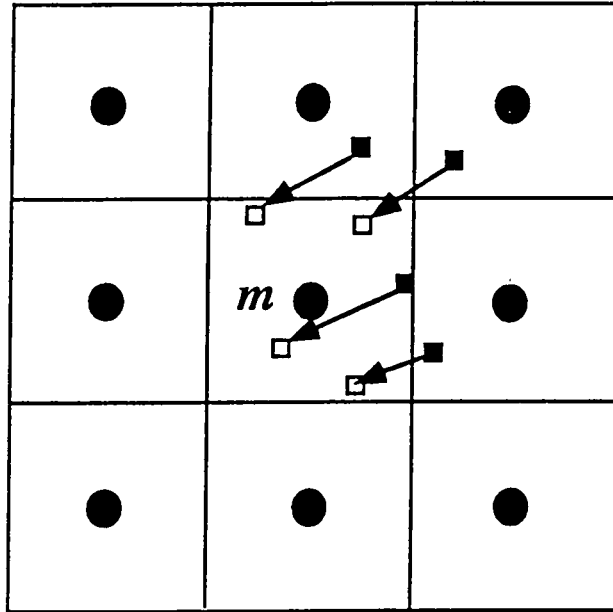
Fig. 3.1. Illustration of the Method Of Characteristics (MOC). A set of moving particles are tracked forward during each time period. An intermediate concentration, equal to the average of the concentrations of all particles in the cell, is assigned to each cell. This intermediate concentration accounts 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 ω 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.,

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

The use of the weighted concentration in equation (3.8) represents an averaged approach because the processes 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 $C_m^{\hat{n}^*}$ and ΔC_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 $(n+1)$. 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):

$$C_m^{n*} = C^n(\mathbf{x}_p) = C^n(\mathbf{x}_m - \mathbf{d}) \qquad (3.9)$$

where

$\mathbf{x}_p$ 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 Δt;

$\mathbf{x}_m$ is the position vector of nodal point m;

$\mathbf{d}$ is the characteristic nodal displacement, or the distance along a particle path from $\mathbf{x}_m$ to $\mathbf{x}_p$;

$C^n(\mathbf{x}_p)$ is the concentration at position $\mathbf{x}_p$ 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

MMOC

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

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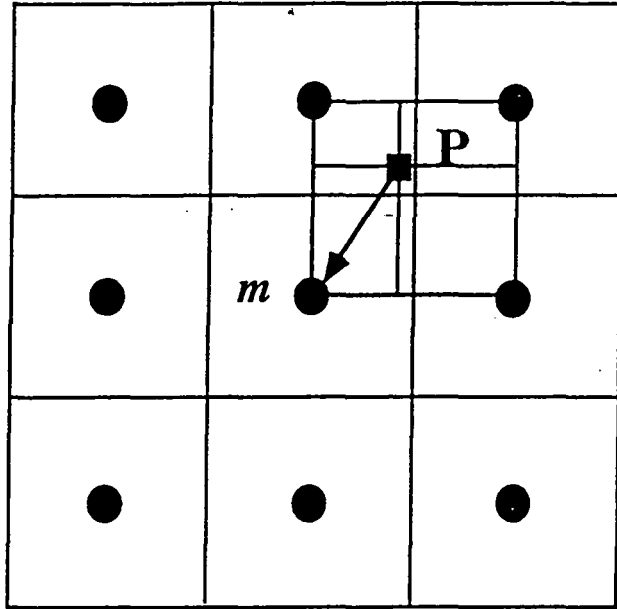
Fig. 3.2. Illustration of the Modified Method Of Characteristics (MMOC). One fictitious particle is placed at each node and tracked backward in time to find its position at the previous time level. The concentration associated with that position is the intermediate concentration due to the effect of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

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. 2.1b 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 offseting much of the advantage of the MMOC technique. 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 tracking 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 from 0 to ∞ 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 (I), columns (J), and layers (K) as illustrated in Fig. 4.1. Following the convention used in Fig. 4.1, the width of cells in the row direction, at a given column, J, is designated Δr_j, the width of cells in the column direction, at a given row, I, is designated Δc_i, and the thickness of cells in a given layer, K, is designated Δv_k. Thus a cell with indices (i,j,k) has a volume of $\Delta r_j \Delta c_i \Delta v_k$.

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, Δr_j along the row direction is equivalent to Δx_j along the x axis; Δc_i along the column direction is equivalent to Δy_i along the y axis; and Δv_k along the layer direction is equivalent to Δz_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

Columns (J)

1   2   3   4   5   6   7   8   9
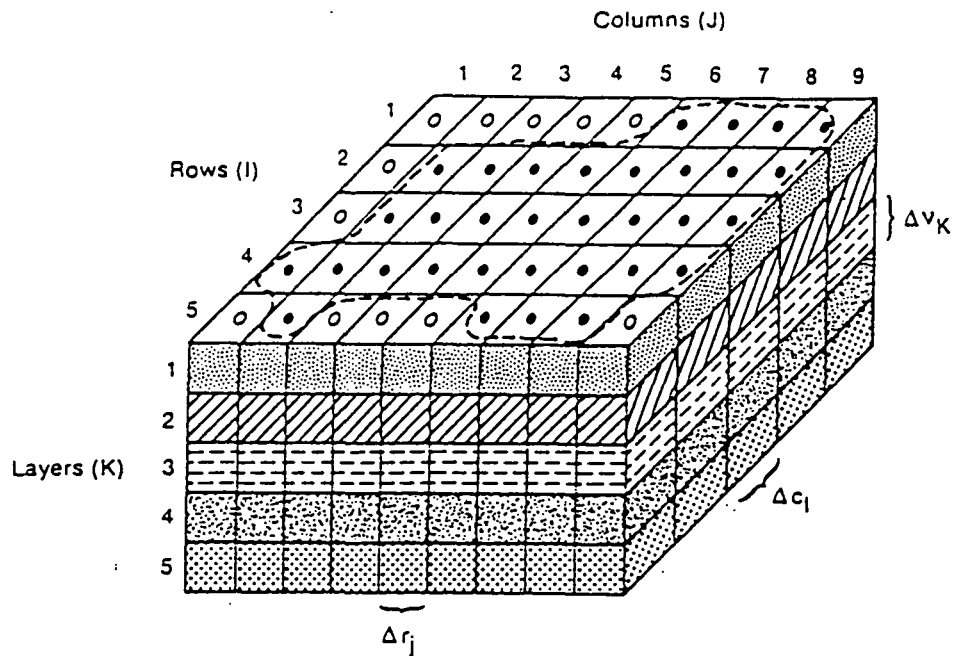
Explanation

———— Aquifer Boundary

•   Active Cell

o   Inactive Cell

Δr_J Dimension of Cell Along the Row Direction. Subscript (J) Indicates the Number of the Column

Δc_I Dimension of Cell Along the Column Direction. Subscript (I) Indicates the Number of the Row

Δv_K 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).
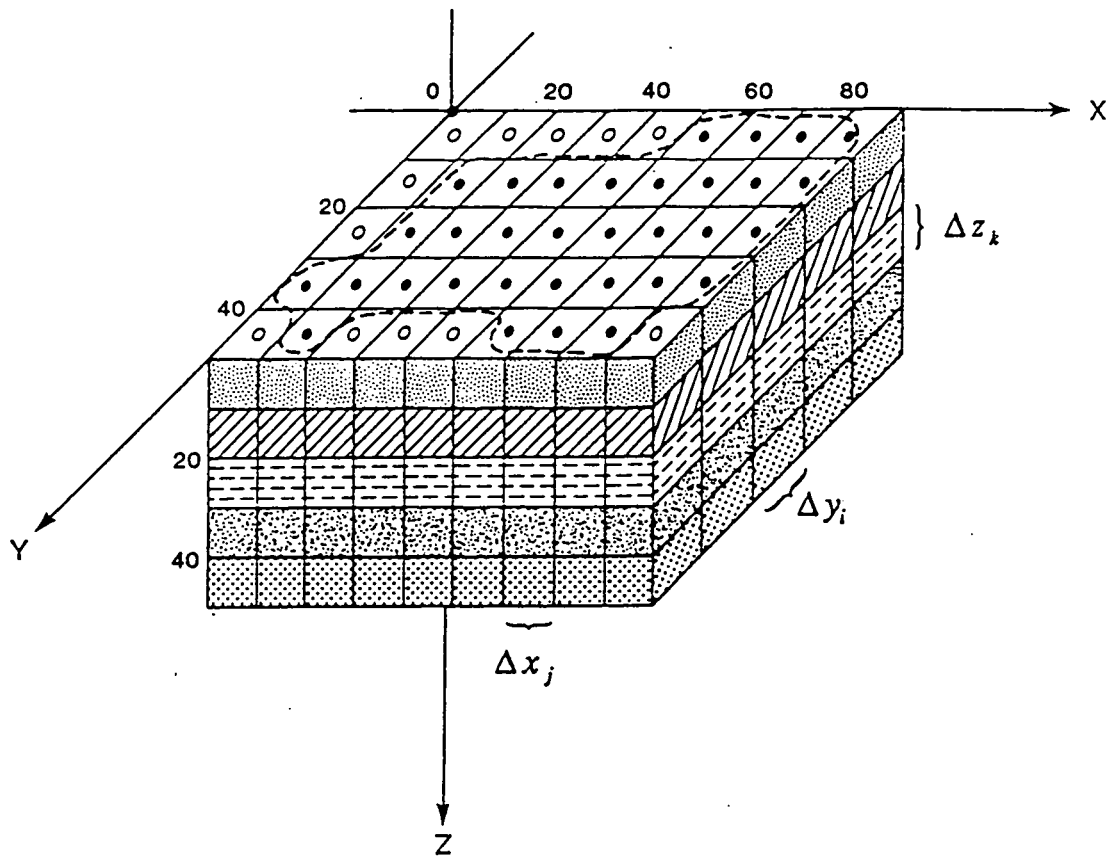
Assuming that:

$\Delta x_j = 10$ 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.

Block-Centered Grid System
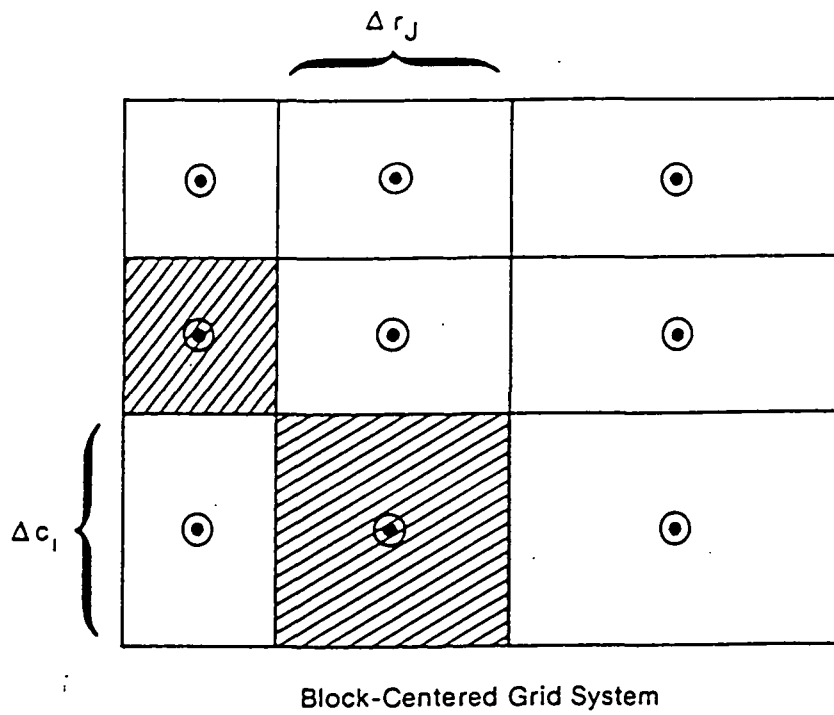
Explanation

⊙   Nodes

———   Grid Lines

///// Cells Associated With
///// Selected Nodes

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

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.

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 time step is normally calculated by the program using the user-specified length of the stress period, 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.
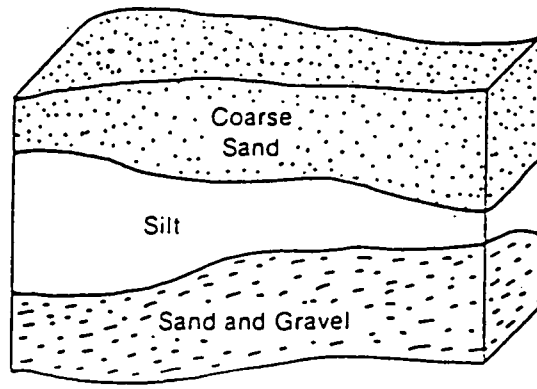
(a) Aquifer Cross Section

Coarse Sand

Silt

Sand and Gravel

Grid Layer 1

Grid Layer 2

Grid Layer 3

Cell Contains Material from Three Stratigraphic Units. All Faces Are Rectangles
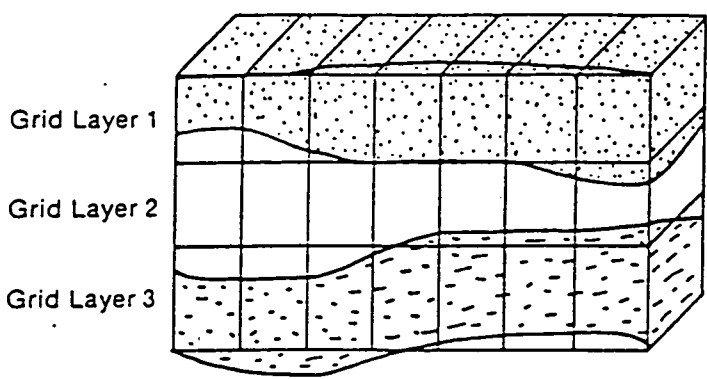
(b) Aquifer Cross Section With Rectilinear Grid Superimposed

Grid Layer 1

Grid Layer 2

Grid Layer 3

Cell Contains Material from Only One Stratigraphic Unit. Faces Are Not Rectangles
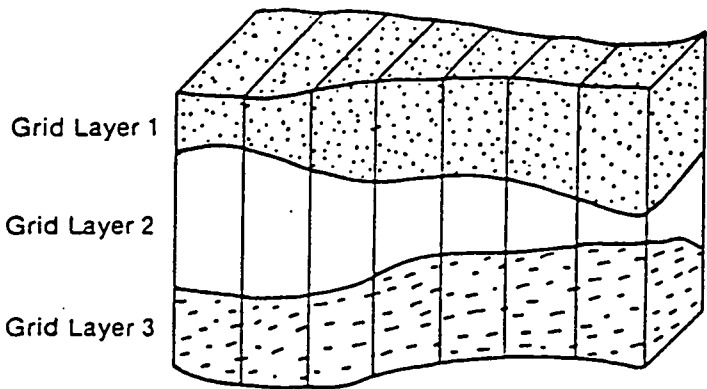
(c) Aquifer Cross Section With Deformed Grid Superimposed

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

(a) Simulation time is divided into Stress Periods and Time Steps
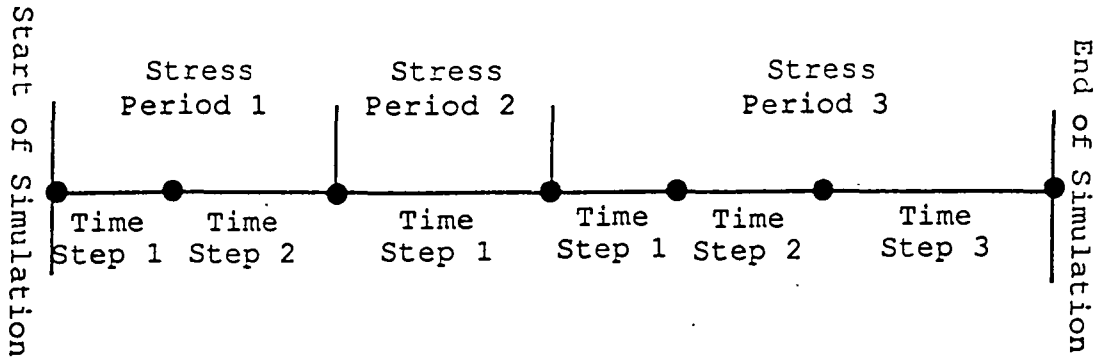
(b) Time Step is further divided into Transport Steps
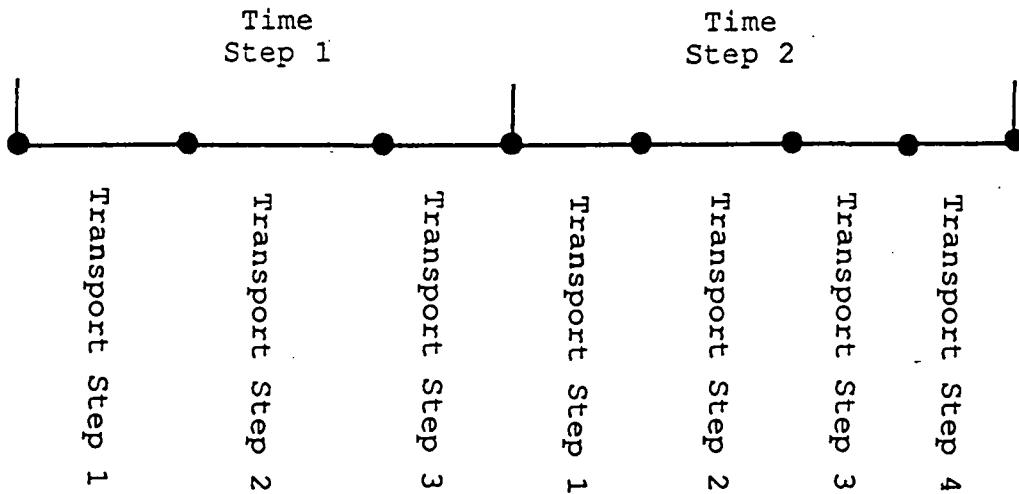
Fig. 4.5. Discretization of simulation time in the transport model.

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

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

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

$x_{j\mp1/2}$ 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

Δx_j is the cell width along the x-axis at cell (i,j,)
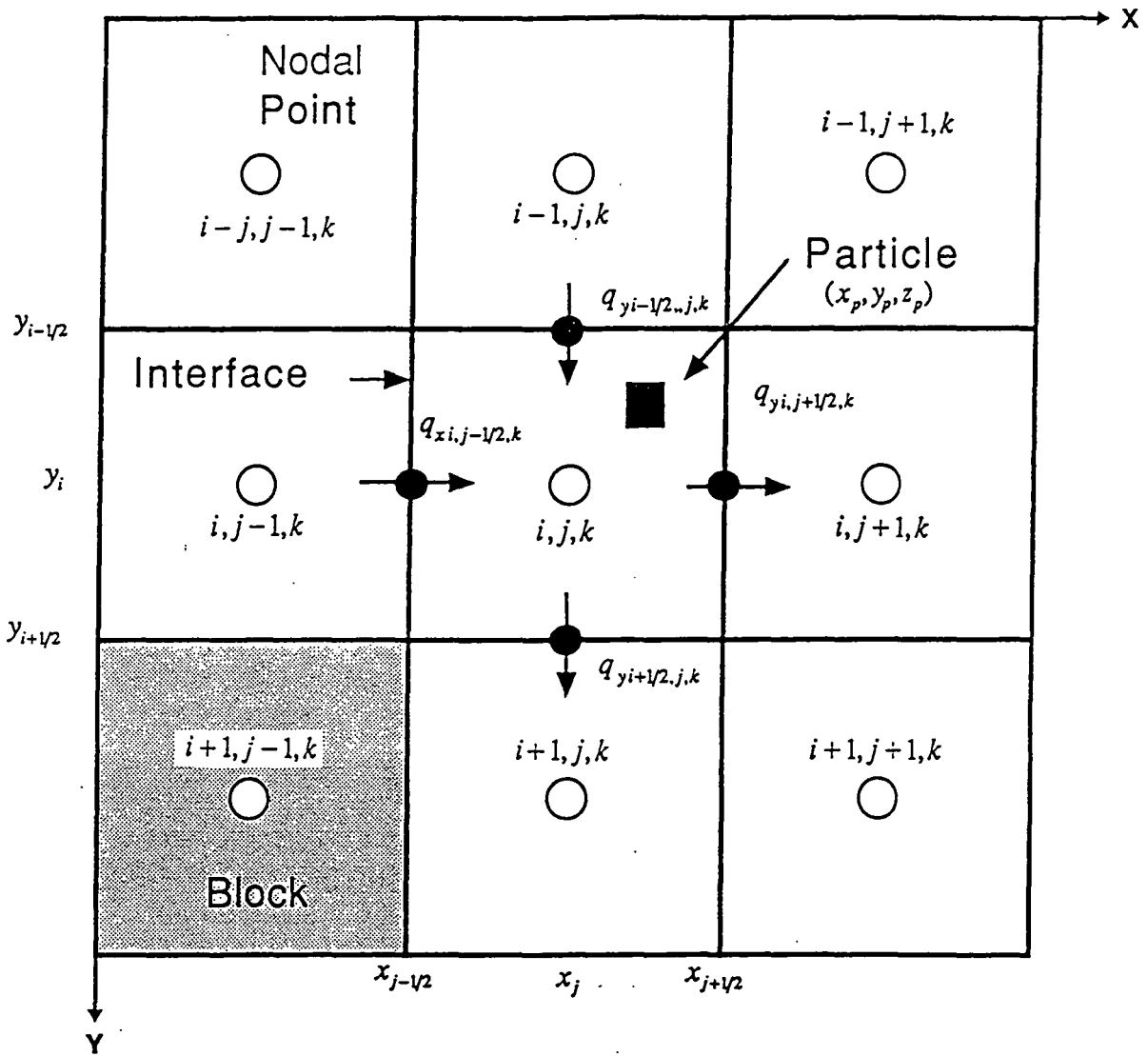
Fig. 4.6. The velocity interpolation scheme used in particle tracking.

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

$$v_x(x_P, y_P, z_P) = \frac{q_x(x_P, y_P, z_P)}{\theta_{i,j,k}} \qquad (4.2)$$

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

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

$$q_y(x_P, y_P, z_P) = (1 - \alpha_y)q_{i-1/2,j,k} + \alpha_y q_{i+1/2,j,k} \qquad (4.3)$$

$$v_y(x_P, y_P, z_P) = \frac{q_y(x_P, y_P, z_P)}{\theta_{i,j,k}} \qquad (4.4)$$

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

$$q_z(x_P, y_P, z_P) = (1 - \alpha_z)q_{i,j,k-1/2} + \alpha_z q_{i,j,k+1/2} \qquad (4.5)$$

$$v_z(x_P, y_P, z_P) = \frac{q_z(x_P, y_P, z_P)}{\theta_{i,j,k}} \qquad (4.6)$$

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):

$$
\begin{cases}
x^{n+1} = x^n + \dfrac{\Delta t}{R} v_x(x^n, y^n, z^n) \\[2mm]
y^{n+1} = y^n + \dfrac{\Delta t}{R} v_y(x^n, y^n, z^n) \\[2mm]
z^{n+1} = z^n + \dfrac{\Delta t}{R} v_z(x^n, y^n, z^n)
\end{cases}
\tag{4.7}
$$

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. Δt is the size of the transport step, which is generally determined from the so-called "Courant condition", or,

$$
|\Delta t| \leq \gamma_c R \, MIN(\frac{\Delta x}{v_x}, \frac{\Delta y}{v_y}, \frac{\Delta z}{v_z})
\tag{4.8}
$$

where γ_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 Δt is positive, and backward if the sign of Δt is negative.

A uniform step size, Δt, 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 Δt 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:

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

where

$$k_1 = \Delta t v_x\left(x^n, y^n, z^n, t^n\right)$$
$$k_2 = \Delta t v_x\left(x^n + k_1/2, y^n + l_1/2, z^n + m_1/2, t^n + \Delta t/2\right)$$
$$k_3 = \Delta t v_x\left(x^n + k_2/2, y^n + l_2/2, z^n + m_2/2, t^n + \Delta t/2\right)$$
$$k_4 = \Delta t v_x\left(x^n + k_3, y^n + l_3, z^n + m_3, t^n + \Delta t\right)$$

$$l_1 = \Delta t v_y\left(x^n, y^n, z^n, t^n\right)$$
$$l_2 = \Delta t v_y\left(x^n + k_1/2, y^n + l_1/2, z^n + m_1/2, t^n + \Delta t/2\right)$$
$$l_3 = \Delta t v_y\left(x^n + k_2/2, y^n + l_2/2, z^n + m_2/2, t^n + \Delta t/2\right)$$
$$l_4 = \Delta t v_y\left(x^n + k_3, y^n + l_3, z^n + m_3, t^n + \Delta t\right)$$

$$m_1 = \Delta t v_z\left(x^n, y^n, z^n, t^n\right)$$
$$m_2 = \Delta t v_z\left(x^n + k_1/2, y^n + l_1/2, z^n + m_1/2, t^n + \Delta t/2\right)$$
$$m_3 = \Delta t v_z\left(x^n + k_2/2, y^n + l_2/2, z^n + m_2/2, t^n + \Delta t/2\right)$$
$$m_4 = \Delta t v_z\left(x^n + k_3, y^n + l_3, z^n + m_3, t^n + \Delta t\right)$$
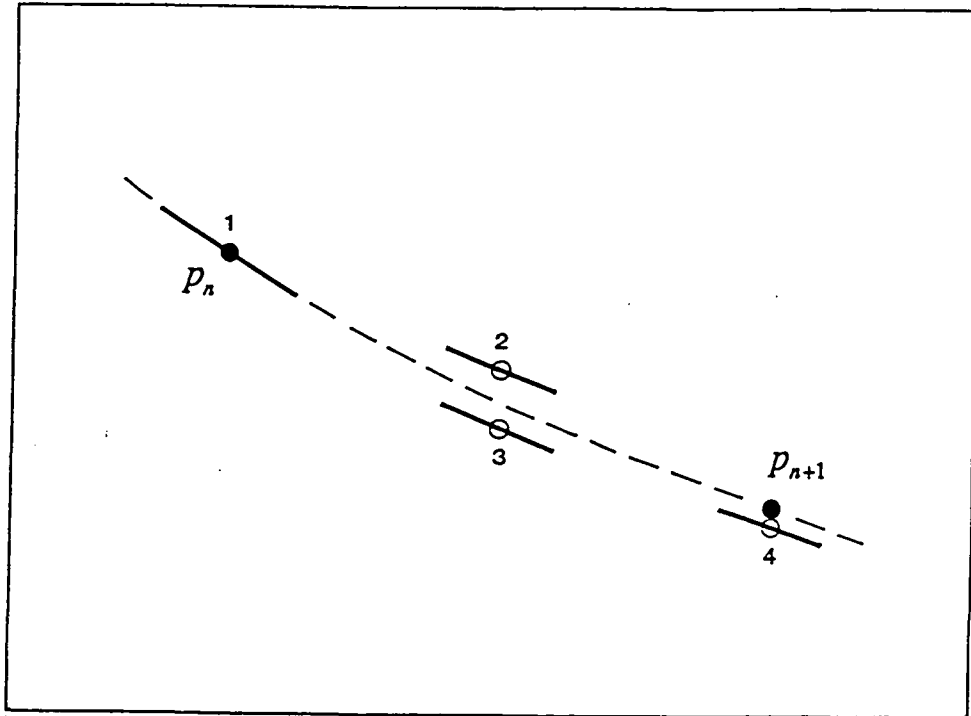
Fig. 4.7. The fourth-order Runge-Kutta method. In each step, the velocity is evaluated four times: once at the initial point, twice at trial midpoints, and once at a trial endpoint. From these velocities a weighted velocity is calculated which is used to compute the final position of the particle (shown 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 (i,j,k);

CMAX is the maximum concentration in the entire grid; and

CMIN 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.,

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

where $NP_{i,j,k}$ 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 NPMAX, 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 illustrates the dynamic particle distribution approach in contrast with the uniform approach in simulating two-dimensional solute transport from a continuous point
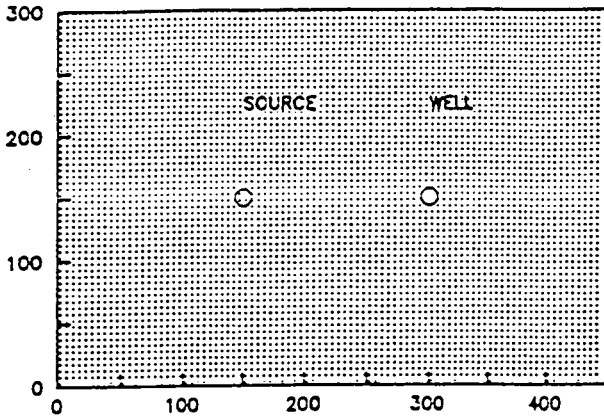
Uniform approach
(5700 particles used)
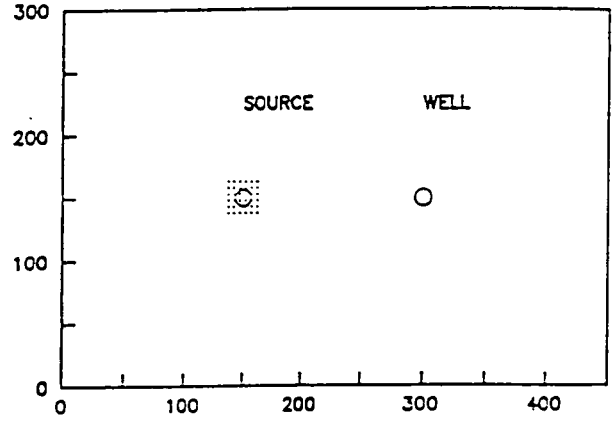
Dynamic approach
(36 particles used)

(b) At time = 365 days
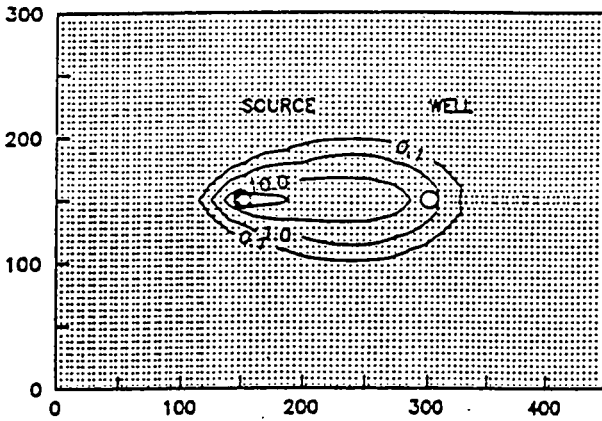
Uniform approach
(5700 particles used)
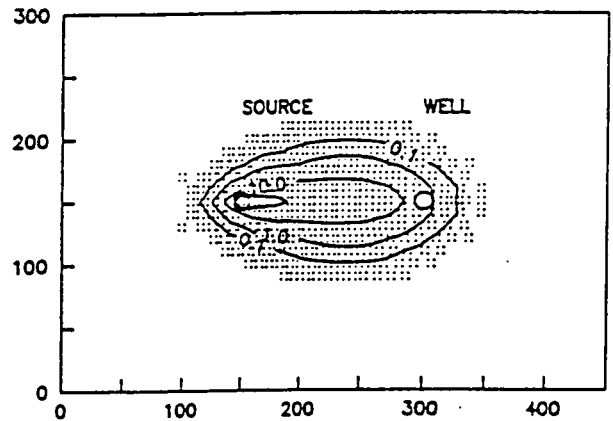
Dynamic approach
(1020 particles used)

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

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.
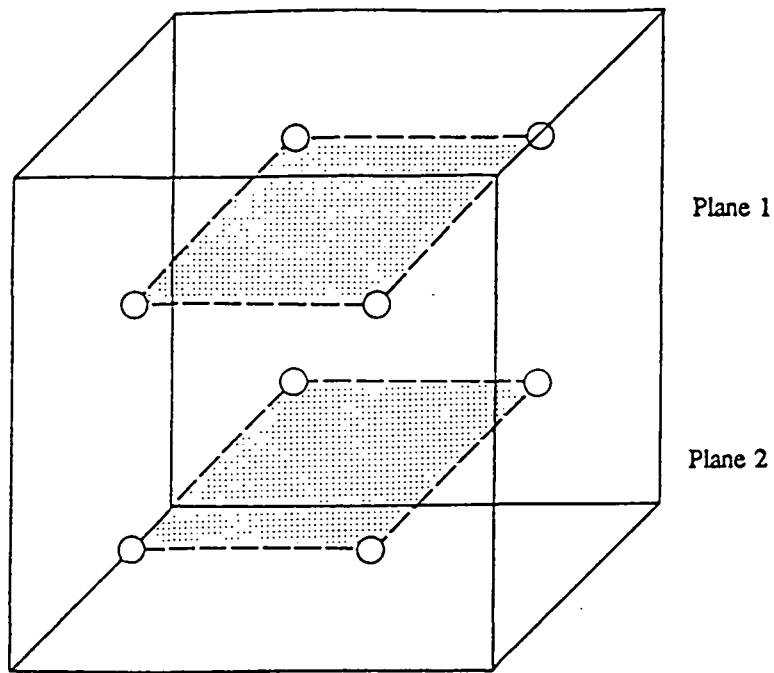
Plane 1

Plane 2

(a) Fixed pattern (8 particles are placed
on two planes within the cell block)
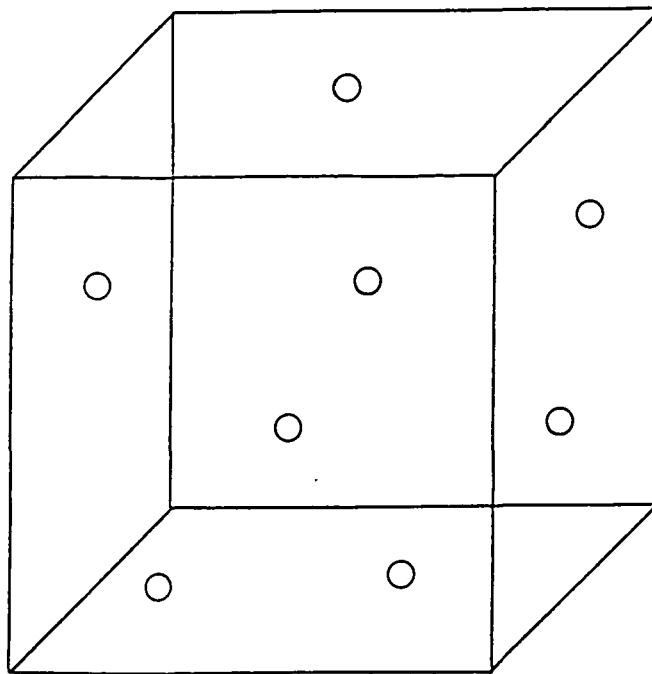
(b) Random pattern (8 particles are placed
randomly within the cell block)

Fig. 4.9. Initial placement of moving particles.

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, Δt, 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, $C_{i,j,k}^{n^*}$, is obtained by accumulating the concentrations of all particles that are located at that cell, divided by the number of particles:

$$C_{i,j,k}^{n^*} = \frac{1}{NP_{i,j,k}} \sum_{l=1}^{NP_{i,j,k}} C_l^n, \quad if \; NP_{i,j,k} > 0 \tag{4.12}$$

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:

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

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:

$$\begin{cases} JP = INT(x_P/\Delta x) + 1 \\ IP = INT(y_P/\Delta y) + 1 \\ KP = INT(z_P/\Delta z) + 1 \end{cases} \tag{4.14}$$

where $INT(x)$ is a FORTRAN function, equal to the truncated value of x; and Δx, Δy, Δz 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. 4.10.
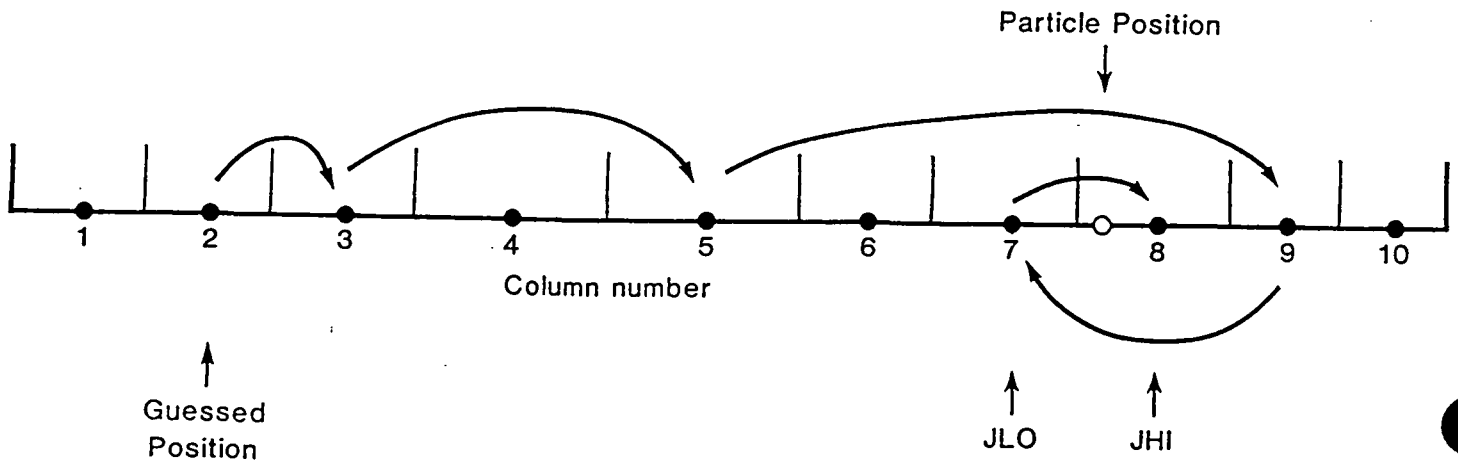
Fig. 4.10. To determine in which cell a particle P is located in an irregular mesh, a searching procedure is first started from a guessed position, either up or down, in increments of one, two, then four, etc., until the desired value is bracketed. Second, a bisection routine is used to bisect the nodal 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.

After the $C_{i,j,k}^{n*}$ 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):

$$C_l^{n+1} = C_l^n + \Delta C^{n+1}_{i,j,k} \tag{4.15}$$

where C_l^{n+1} is the concentration of the lth particle which is located at cell (i,j,k) at the new time level. If $\Delta C^{n+1}_{i,j,k}$ is positive, equation (4.15) is applied directly. However, if $\Delta C^{n+1}_{i,j,k}$ 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:

$$C_l^{n+1} = C_l^n \times (1 + \Delta C^{n+1}_{i,j,k} / C^{n*}_{i,j,k}) \tag{4.16}$$

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 with that position, denoted as $(\hat{x}, \hat{y}, \hat{z})$, is the concentration of the cell due to advection alone over the time increment Δt.

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, $\hat{y}$ between y_{i-1} and y_i, and $\hat{z}$ between z_{k-1} and z_k (also see Fig. 4.11):

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

where ω_x, ω_y and ω_z are interpolation factors as given below:

$$
\begin{cases}
\omega_x = \dfrac{\hat{x}-x_{j-1}}{0.5\Delta x_j + 0.5\Delta x_{j-1}} \\[2ex]
\omega_y = \dfrac{\hat{y}-y_{i-1}}{0.5\Delta y_i + 0.5\Delta y_{i-1}} \\[2ex]
\omega_z = \dfrac{\hat{z}-z_{k-1}}{0.5\Delta z_k + 0.5\Delta z_{k-1}}
\end{cases}
\tag{4.18}
$$

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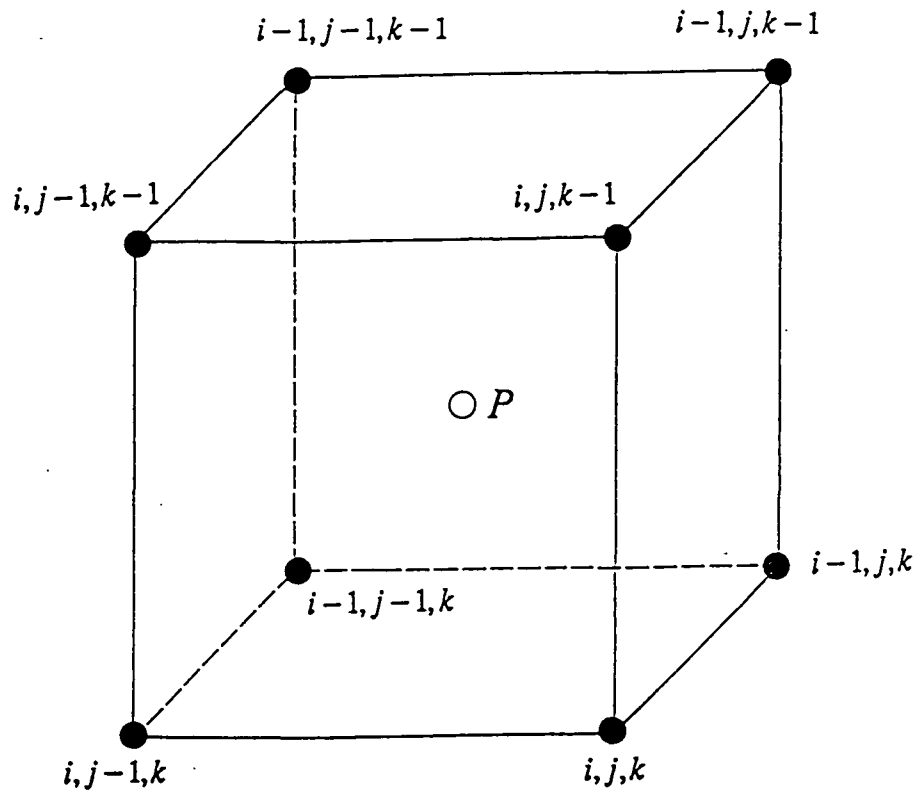
Fig. 4.11. Interpolation of the concentration at point P from the concentrations at neighboring nodes using the trilinear scheme in three dimensions.

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 Δt, 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:

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

where d_l is the distance between the nodal point and the position where the lth 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:

$$C_{i,j,k}^{n^*} = C_{i,j,k}^n \qquad (4.20)$$

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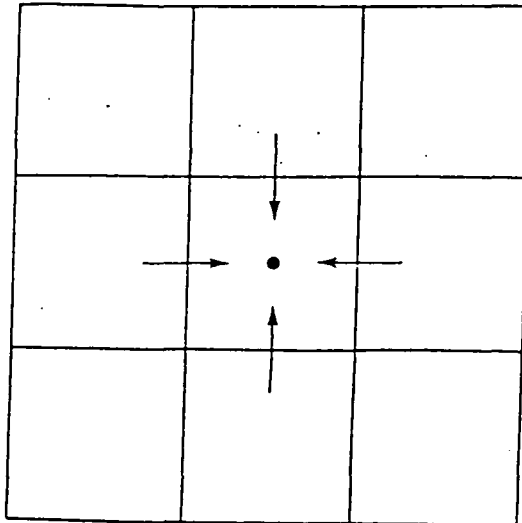
(a) At a sink cell with inward gradients
on all interfaces
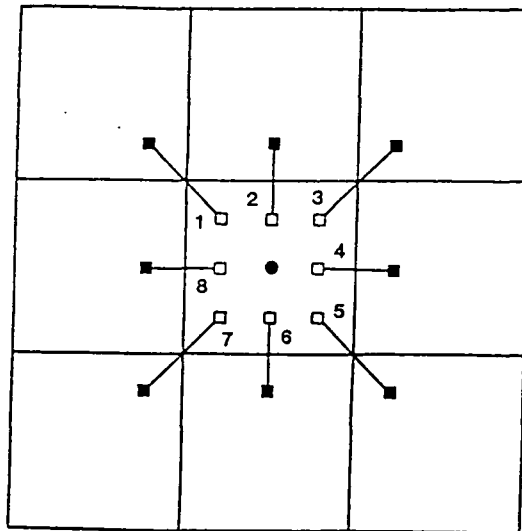
(b) Instead of placing one single particle
at the node, multiple particles are placed
and tracked backward. In this example,
8 particles distributed with a fixed pattern
are used. However, both the number and the
pattern can be changed in the user-specified
options.

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:

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

where $|v_i|$ is the magnitude of the seepage velocity component; Δx_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 $DCHMOC$:

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

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 ∞ 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, $\hat{C}^{n}_{i,j,k}$, is calculated based on $C^{n*}_{i,j,k}$ and the concentration at the old time level $C^{n}_{i,j,k}$:

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

The weighted concentration $\hat{C}^{n}_{i,j,k}$ 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):

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

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

$$\Delta C_{i,j,k}^{n+1} = \frac{\Delta t}{R_{i,j,k}^n} \left\{ D_{xx_{i,j+1/2,k}} \frac{C_{i,j+1,k}^{\hat{}} - C_{i,j,k}^{\hat{}}}{\Delta x_j (0.5\Delta x_j + 0.5\Delta x_{j+1})} - D_{xx_{i,j-1/2,k}} \frac{C_{i,j,k}^{\hat{}} - C_{i,j-1,k}^{\hat{}}}{\Delta x_j (0.5\Delta x_{j-1} + 0.5\Delta x_j)} \right.$$

$$+ D_{xy_{i,j+1/2,k}} \frac{\omega_{x_{j+1/2}} C_{i+1,j,k}^{\hat{}} + (1-\omega_{x_{j+1/2}}) C_{i+1,j+1,k}^{\hat{}} - \omega_{x_{j+1/2}} C_{i-1,j,k}^{\hat{}} - (1-\omega_{x_{j+1/2}}) C_{i-1,j+1,k}^{\hat{}}}{\Delta x_j (0.5\Delta y_{i-1} + \Delta y_i + 0.5\Delta y_{i+1})}$$

$$- D_{xy_{i,j-1/2,k}} \frac{\omega_{x_{j-1/2}} C_{i+1,j,k}^{\hat{}} + (1-\omega_{x_{j-1/2}}) C_{i+1,j,k}^{\hat{}} - \omega_{x_{j-1/2}} C_{i-1,j-1,k}^{\hat{}} - (1-\omega_{x_{j-1/2}}) C_{i-1,j,k}^{\hat{}}}{\Delta x_j (0.5\Delta y_{i-1} + \Delta y_i + 0.5\Delta y_{i+1})}$$

$$+ D_{xz_{i,j+1/2,k}} \frac{\omega_{x_{j+1/2}} C_{i,j,k+1}^{\hat{}} + (1-\omega_{x_{j+1/2}}) C_{i,j+1,k+1}^{\hat{}} - \omega_{x_{j+1/2}} C_{i,j,k-1}^{\hat{}} - (1-\omega_{x_{j+1/2}}) C_{i,j+1,k-1}^{\hat{}}}{\Delta x_j (0.5\Delta z_{k-1} + \Delta z_k + 0.5\Delta z_{k+1})}$$

$$- D_{xz_{i,j-1/2,k}} \frac{\omega_{x_{j-1/2}} C_{i,j-1,k+1}^{\hat{}} + (1-\omega_{x_{j-1/2}}) C_{i,j,k+1}^{\hat{}} - \omega_{x_{j-1/2}} C_{i,j-1,k-1}^{\hat{}} - (1-\omega_{x_{j-1/2}}) C_{i,j,k-1}^{\hat{}}}{\Delta x_j (0.5\Delta z_{k-1} + \Delta z_k + 0.5\Delta z_{k+1})}$$

$$+ D_{yx_{i+1/2,j,k}} \frac{\omega_{y_{i+1/2}} C_{i,j+1,k}^{\hat{}} + (1-\omega_{y_{i+1/2}}) C_{i+1,j+1,k}^{\hat{}} - \omega_{y_{i+1/2}} C_{i,j-1,k}^{\hat{}} - (1-\omega_{y_{i+1/2}}) C_{i+1,j-1,k}^{\hat{}}}{\Delta y_i (0.5\Delta x_{j-1} + \Delta x_j + 0.5\Delta x_{j+1})}$$

$$- D_{yx_{i-1/2,j,k}} \frac{\omega_{y_{i-1/2}} C_{i-1,j+1,k}^{\hat{}} + (1-\omega_{y_{i-1/2}}) C_{i,j+1,k}^{\hat{}} - \omega_{y_{i-1/2}} C_{i-1,j-1,k}^{\hat{}} - (1-\omega_{y_{i-1/2}}) C_{i,j-1,k}^{\hat{}}}{\Delta y_i (0.5\Delta x_{j-1} + \Delta x_j + 0.5\Delta x_{j+1})}$$

$$+ D_{yy_{i+1/2,j,k}} \frac{C_{i+1,j,k}^{\hat{}} - C_{i,j,k}^{\hat{}}}{\Delta y_i (0.5\Delta y_i + 0.5\Delta y_{i+1})} - D_{yy_{i-1/2,j,k}} \frac{C_{i,j,k}^{\hat{}} - C_{i-1,j,k}^{\hat{}}}{\Delta y_i (0.5\Delta y_{i-1} + 0.5\Delta y_i)}$$

$$+ D_{yz_{i+1/2,j,k}} \frac{\omega_{y_{i+1/2}} C_{i,j,k+1}^{\hat{}} + (1-\omega_{y_{i+1/2}}) C_{i+1,j,k+1}^{\hat{}} - \omega_{y_{i+1/2}} C_{i,j,k-1}^{\hat{}} - (1-\omega_{y_{i+1/2}}) C_{i+1,j,k-1}^{\hat{}}}{\Delta y_i (0.5\Delta z_{k-1} + \Delta z_k + 0.5\Delta z_{k+1})}$$

$$- D_{yz_{i-1/2,j,k}} \frac{\omega_{y_{i-1/2}} C_{i-1,j,k+1}^{\hat{}} + (1-\omega_{y_{i-1/2}}) C_{i,j,k+1}^{\hat{}} - \omega_{y_{i-1/2}} C_{i-1,j,k-1}^{\hat{}} - (1-\omega_{y_{i-1/2}}) C_{i,j,k-1}^{\hat{}}}{\Delta y_i (0.5\Delta z_{k-1} + \Delta z_k + 0.5\Delta z_{k+1})}$$

$$+ D_{zx_{i,j,k+1/2}} \frac{\omega_{z_{k+1/2}} C_{i,j+1,k}^{\hat{}} + (1-\omega_{z_{k+1/2}}) C_{i,j+1,k+1}^{\hat{}} - \omega_{z_{k+1/2}} C_{i,j-1,k}^{\hat{}} - (1-\omega_{z_{k+1/2}}) C_{i,j-1,k+1}^{\hat{}}}{\Delta z_k (0.5\Delta x_{j-1} + \Delta x_j + 0.5\Delta x_{j+1})}$$

$$- D_{zx_{i,j,k-1/2}} \frac{\omega_{z_{k-1/2}} C_{i,j+1,k-1}^{\hat{}} + (1-\omega_{z_{k-1/2}}) C_{i,j+1,k}^{\hat{}} - \omega_{z_{k-1/2}} C_{i,j-1,k-1}^{\hat{}} - (1-\omega_{z_{k-1/2}}) C_{i,j-1,k}^{\hat{}}}{\Delta z_k (0.5\Delta x_{j-1} + \Delta x_j + 0.5\Delta x_{j+1})}$$

$$+ D_{zy_{i,j,k+1/2}} \frac{\omega_{z_{k+1/2}} C_{i+1,j,k}^{\hat{}} + (1-\omega_{z_{k+1/2}}) C_{i+1,j,k+1}^{\hat{}} - \omega_{z_{k+1/2}} C_{i-1,j,k}^{\hat{}} - (1-\omega_{z_{k+1/2}}) C_{i-1,j,k+1}^{\hat{}}}{\Delta z_k (0.5\Delta y_{i-1} + \Delta y_i + 0.5\Delta y_{i+1})}$$

$$+ D_{zy_{i,j,k-1/2}} \frac{\omega_{z_{k-1/2}} C_{i+1,j,k-1}^{\hat{}} + (1-\omega_{z_{k-1/2}}) C_{i+1,j,k}^{\hat{}} - \omega_{z_{k-1/2}} C_{i-1,j,k-1}^{\hat{}} - (1-\omega_{z_{k-1/2}}) C_{i-1,j,k}^{\hat{}}}{\Delta z_k (0.5\Delta y_{i-1} + \Delta y_i + 0.5\Delta y_{i+1})}$$

$$\left. + D_{zz_{i,j,k+1/2}} \frac{C_{i,j,k+1}^{\hat{}} - C_{i,j,k}^{\hat{}}}{\Delta z_k (0.5\Delta z_k + 0.5\Delta z_{k+1})} - D_{zz_{i,j,k-1/2}} \frac{C_{i,j,k}^{\hat{}} - C_{i,j,k-1}^{\hat{}}}{\Delta z_k (0.5\Delta z_{k-1} + 0.5\Delta z_k)} \right\}$$

(4.25)

---

where

ΔC_{DSP}^{n+1} is the concentration change due to dispersion 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;

ω_x, ω_y and ω_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 respective directions.

If the grid 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:

$$
\begin{cases}
\omega_{x_{j+1/2}} = \dfrac{\Delta x_{j+1}}{\Delta x_j + \Delta x_{j+1}} \\[2mm]
\omega_{x_{j+1/2}} = \dfrac{\Delta y_{j+1}}{\Delta y_j + \Delta y_{j+1}} \\[2mm]
\omega_{z_{k+1/2}} = \dfrac{\Delta z_{k+1}}{\Delta z_k + \Delta z_{k+1}}
\end{cases}
\qquad (4.26)
$$

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):

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

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

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

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

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 cells (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:

$$D_{xx_{i,j+1/2,k}} = \alpha_{L_{i,j+1/2,k}}v_{x_{i,j+1/2,k}}^2/v_{i,j+1/2,k} + \alpha_{TH_{i,j+1/2,k}}v_{y_{i,j+1/2,k}}^2/v_{i,j+1/2,k}$$
$$+ \alpha_{TV_{i,j+1/2,k}}v_{z_{i,j+1/2,k}}^2/v_{i,j+1/2,k} + D_{m_{i,j+1/2,k}} \tag{4.27h}$$

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

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

Similarly, the components of 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.
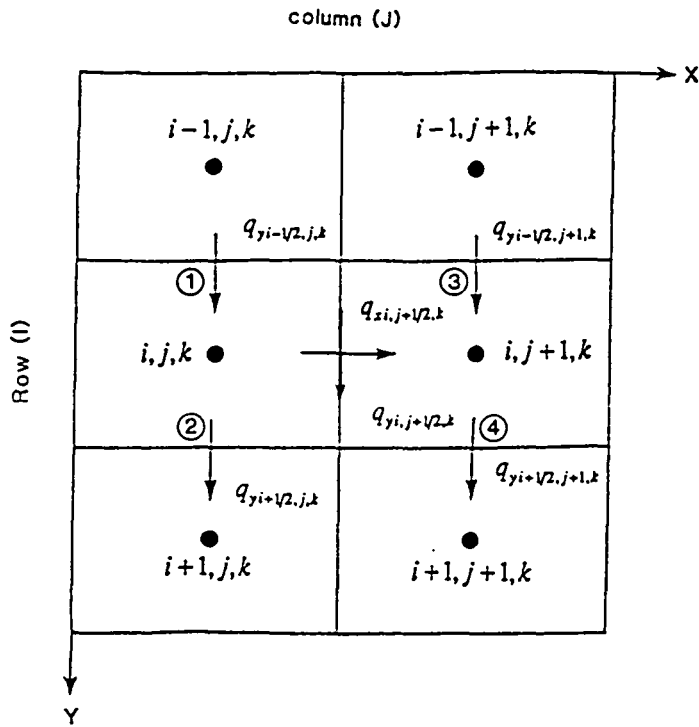
q_x at the interface between (i,j,k) and $(i,j+1,k)$ is directly known from the flow model; q_y at the interface between (i,j,k) and $(i,j+1,k)$ is interpolated from values at interfaces 1, 2, 3 and 4 in the y direction.
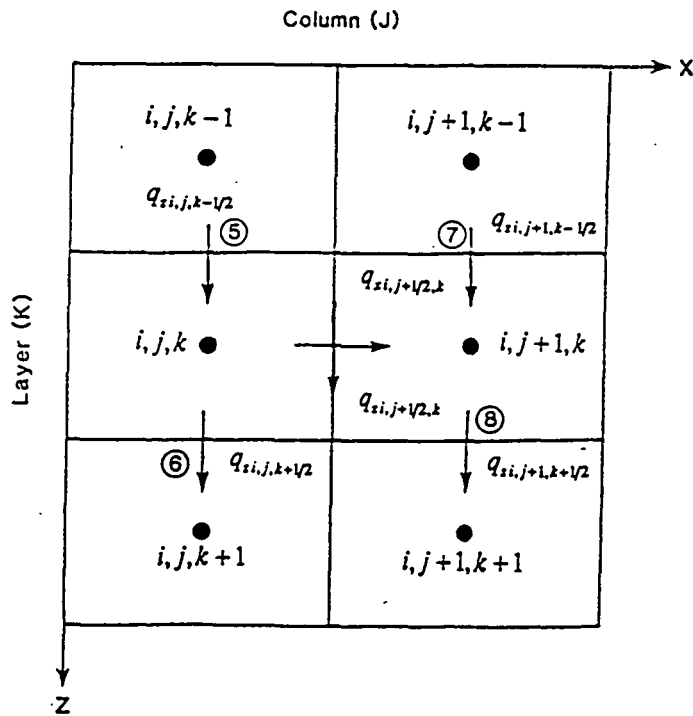
q_z at the interface between (i,j,k) and $(i,j+1,k)$ is interpolated from values at interfaces 5, 6, 7 and 8 in the y direction.

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

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:

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

In the MT3D transport model, equation 4.28 is calculated for each active cell and the minimum Δt 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:

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

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, $C^n_{Si,j,k}$, that is,

$$\frac{\Delta C^{n+1}_{SSM\,i,j,k}}{C^{\hat{n}}_{i,j,k} - C^n_{Si,j,k}} \leq 1, \quad C^{\hat{n}}_{i,j,k} \neq C^n_{Si,j,k}$$

(4.31)

or

$$\Delta t \leq \left| \frac{R^n_{i,j,k}\,\theta_{i,j,k}}{q^n_{Si,j,k}} \right|$$

(4.32)

where $q^n_{Si,j,k}$ 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 isotherm, the retardation factor is calculated as:

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

(4.33)

where ρ_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:

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

(4.34)

where S_1 represents the Freundlich constant K_f and S_2 represents the Freundlich exponent a

(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:

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

(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:

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

(4.36)

which reflects the loss of both solute and sorbed mass, or masses gained if the sign of the rate

constants, λ_1 and λ_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:

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

(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 $\bar{C}^{\hat{}}{}_{i,j,k}$ is the sorbed concentration in equilibrium with solute concentration $C^{\hat{}}{}_{i,j,k}$ in the same cell:

$$\begin{cases} \bar{C}^{\hat{}}{}_{i,j,k} = S_1 C^{\hat{}}{}_{i,j,k}, & \text{for Linear isotherm;} \\[2mm] \bar{C}^{\hat{}}{}_{i,j,k} = S_1 C^{\hat{}}{}_{i,j,k}^{(S_2-1)}, & \text{for Freundlich isotherm;} \\[2mm] \bar{C}^{\hat{}}{}_{i,j,k} = \dfrac{S_1 S_2 C^{\hat{}}{}_{i,j,k}}{1 + S_1 C^{\hat{}}{}_{i,j,k}}, & \text{for Langmuir isotherm.} \end{cases} \tag{4.38}$$

The stability criterion associated with this explicit scheme is,

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

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, general-head-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

Injection Well

Flow Rate (Q)=1,
Concentration (C)=1

Uniform flow

C=1   C=0   C=0   C=0

Cell 1   Cell 2   Cell 3   Cell 4
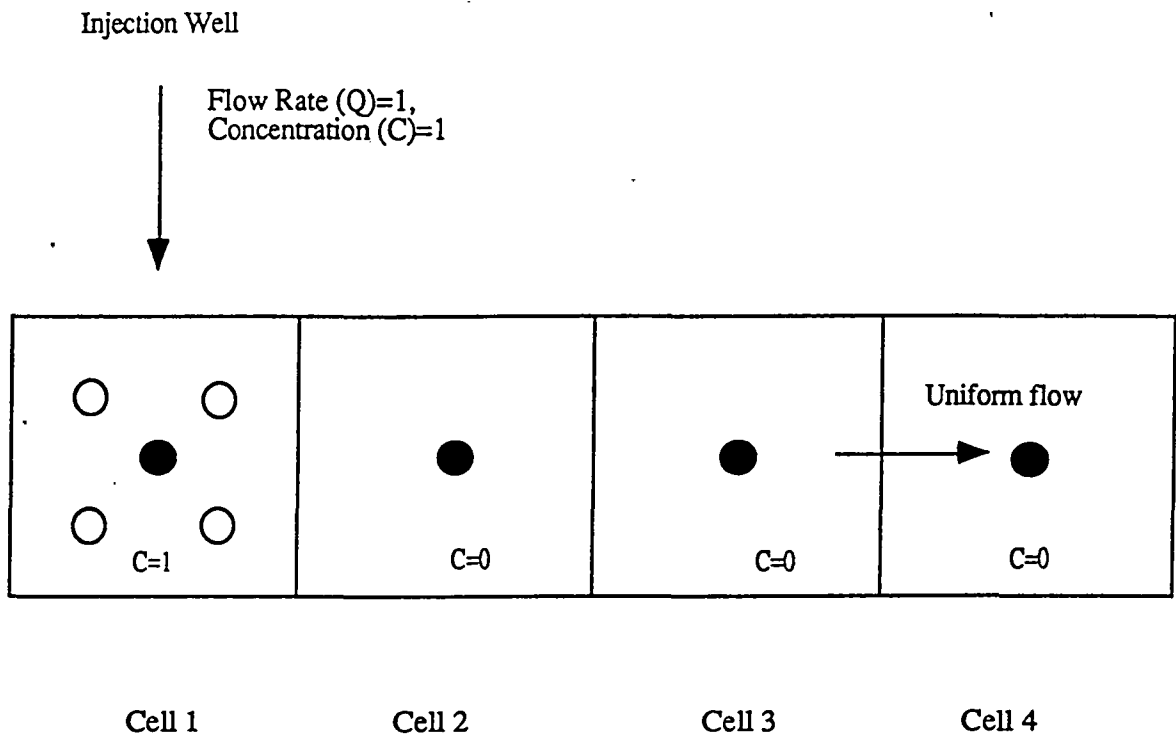
Fig. 4.14. Example of mass balance discrepancy due to discrete nature of moving particle methods.

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 is generally not very meaningful to look at the 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 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:

$$\frac{\partial}{\partial x_i}(v_i C) = \frac{v_{xi,j+1/2,k}\, C_{i,j+1/2,k} - v_{xi,j-1/2,k}\, C_{i,j-1/2,k}}{\Delta x_j}$$

$$+\frac{v_{yi+1/2,j,k}\, C_{i+1/2,j,k} - v_{xi-1/2,j,k}\, C_{i-1/2,j,k}}{\Delta y_i}$$

$$+\frac{v_{zi,j,k+1/2}\, C_{i,j,k+1/2} - v_{zi,j,k-1/2}\, C_{i,j,k-1/2}}{\Delta z_k} \tag{4.41}$$

where

$$C_{i,j+1/2,k} = \begin{cases} C_{i,j,k}, & \text{if } v_{xi,j+1/2,k} > 0 \\ C_{i,j+1,k}, & \text{if } v_{xi,j+1/2,k} < 0 \end{cases}$$

$$C_{i+1/2,j,k} = \begin{cases} C_{i,j,k}, & \text{if } v_{yi+1/2,j,k} > 0 \\ C_{i+1,j,k}, & \text{if } v_{yi+1/2,j,k} < 0 \end{cases}$$

$$C_{i,j,k+1/2} = \begin{cases} C_{i,j,k}, & \text{if } v_{zi,j,k+1/2} > 0 \\ C_{i,j,k+1}, & \text{if } v_{zi,j,k+1/2} < 0 \end{cases}$$

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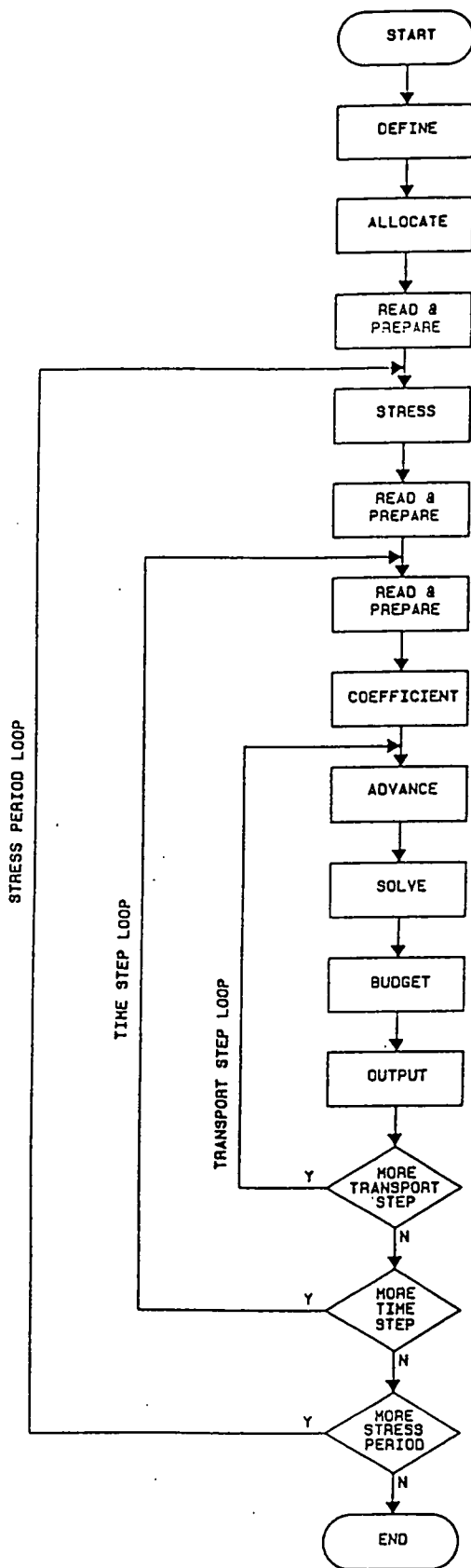
Fig. 5.1. General procedures for a typical transport simulation.

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 (RCT).

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 within its respective package.

Packages

Procedures —

Procedure	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					

Stress period loop

Time step loop

Transport step loop

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 Transport	BTN	Handles basic tasks that are required by the entire 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 Interface	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 Reactions	RCT	Solves the concentration change due to chemical 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.
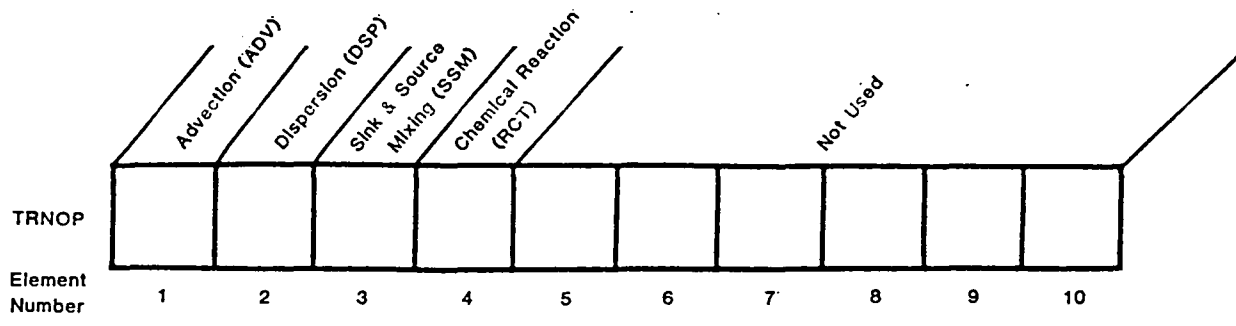
Sample TRNOP Input Record

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.

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=1, 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: MT3D.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=11, IUCN=12, IOBS=13, IMAS=14, ICNF=15)

where

IOUT is the unit number for the Standard Output File;

IUCN is the unit number for the Unformatted 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, if 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 IX 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 time 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.
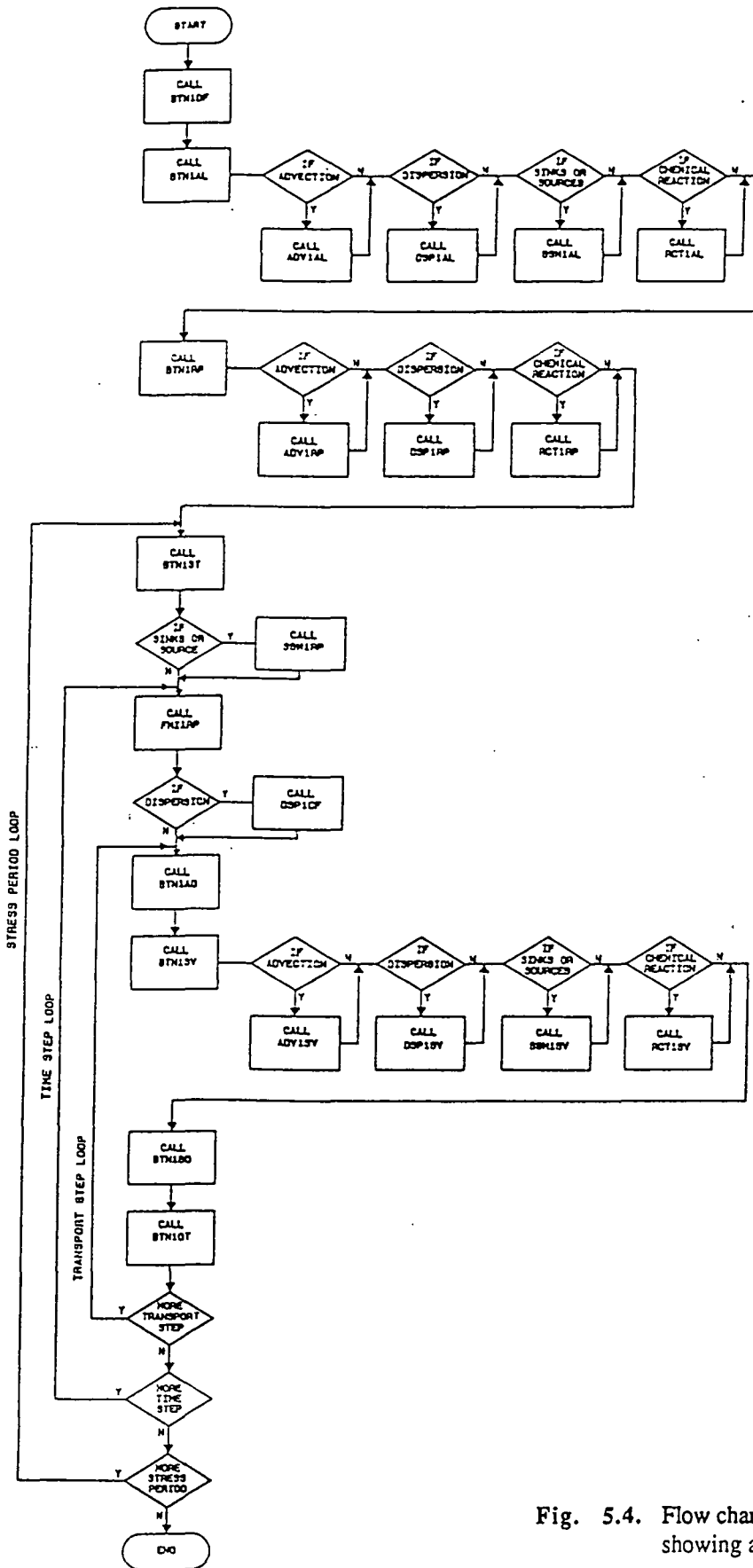
Fig. 5.4. Flow chart for the main program showing all primary modules.

5.5.2 Basic Transport Package -- *MTBTN1*

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

BTN1DF - Define the simulation problem by reading the number of layers, rows, columns and stress periods as well as the transport options to be used;

BTN1AL - Allocate space for basic data arrays needed by the model as a whole;

BTN1RP - Read and prepare basic data arrays used by the entire model;

BTN1ST - Read stress period timing information;

BTN1AD - Determine an appropriate stepsize for each transport step;

BTN1SV - Update cell concentrations and prepare for simulation of the next step;

BTN1BD - Prepare global mass balance information;

BTN1OT - Print or save simulation results according to the user-specified options.

5.5.3 Flow Model Interface Package -- *MTFMI1*

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

FMI1RP1 - 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.

FMI1RP2 - 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 -- *MTADV1*

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

ADV1AL - Allocate space for data arrays needed by the Advection Package;

ADV1RP - Read and prepare input data needed for solving the advection term;

ADV1SV - 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 -- *MTDSP1*

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

DSP1AL - Allocate space for data arrays needed by the Dispersion Package;

DSP1RP - Read and prepare dispersion parameters;

DSP1CF - Calculate components of the hydrodynamic dispersion coefficient;

DSP1SV - Solve the dispersion term using the explicit finite difference formulation;

5.5.6 Sink & Source Mixing Package -- *MTSSM1*

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 -- *MTRCT1*

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 RCT1RP and RCT1SV use the following secondary module:

RFCOEF: Calculate retardation factor for linear or non-linear sorption isotherms.

5.5.8 Utility Package -- *MTUTL1*

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.

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 (IARRAY):

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 (I1), last row (I2), first column (J1), 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(1),.ZV(2),........., ZV(NZONE)   (free format)
A(NCOL,NROW)   (using format FMTIN)

The zonal format for IARRAY:
NZONE   (free format)
IZV(1), 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>0, it is the unit number on which the external file is read using the format specified in FMTIN.

If IREAD<0, 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.

CNSTNT/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 IPRN code.
(After McDonald and Harbaugh, 1988)

IPRN	RARRAY	IARRAY
0	10G11.4	10I11
1	11G10.3	6I1
2	9G13.6	4I2
3	15F7.1	3I3
4	15F7.2	25I4
5	15F7.3	20I5
6	15F7.4	
7	20F5.0	
8	20F5.1	
9	20F5.2	
10	20F5.3	
11	20F5.4	
12	10G11.4	

		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.

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 flow model. 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 unformatted 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. The 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 following to add the LKMT package into MODFLOW:

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

   ```
   CALL BAS1OC (...)
   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 and cell-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: 4I10
          • 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(1) 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 Δx). Enter one value for each
                column in the grid.

A8   Array: DELC(NROW)
      Reader: RARRAY
              - DELC is the cell width along columns (or Δy). 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<0, 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>0, 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 for print-formats are the same as those listed in Table 6.1.

  If IFMTCN>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: I10

       • 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≤0, 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: DT0, MXSTRN

　　　Format: F10.0, I10

- DT0 is the user-specified transport stepsize. The program will 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.
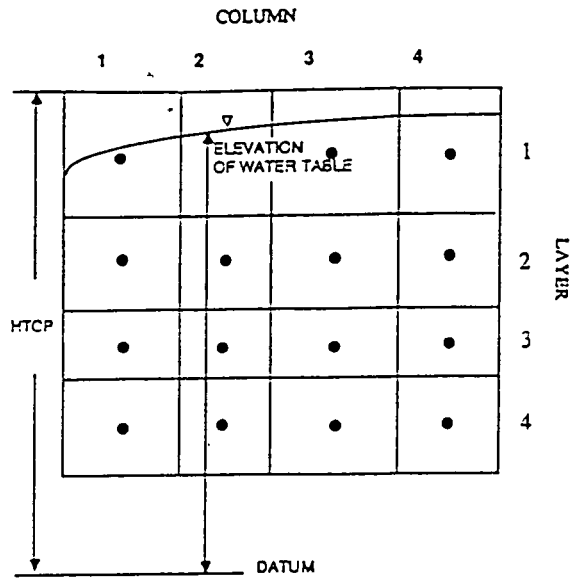
(a) Array HTOP for unconfined aquifer
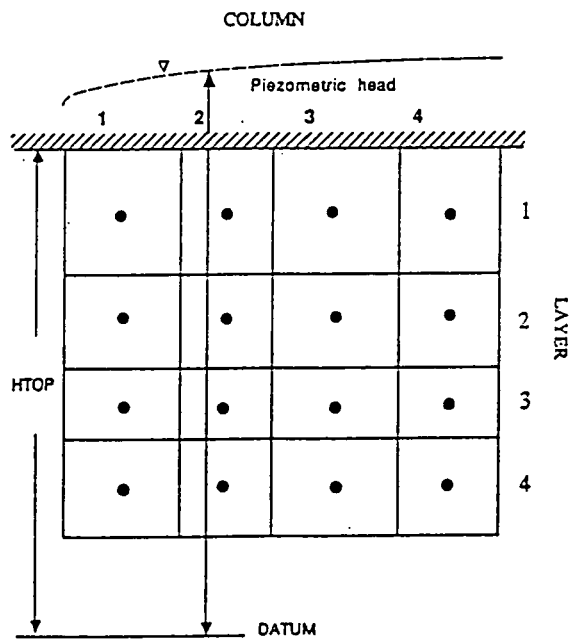
(b) Array HTOP for confined aquifer

Fig. 6.2. · Illustration of array HTOP for unconfined and confined aquifer layers.
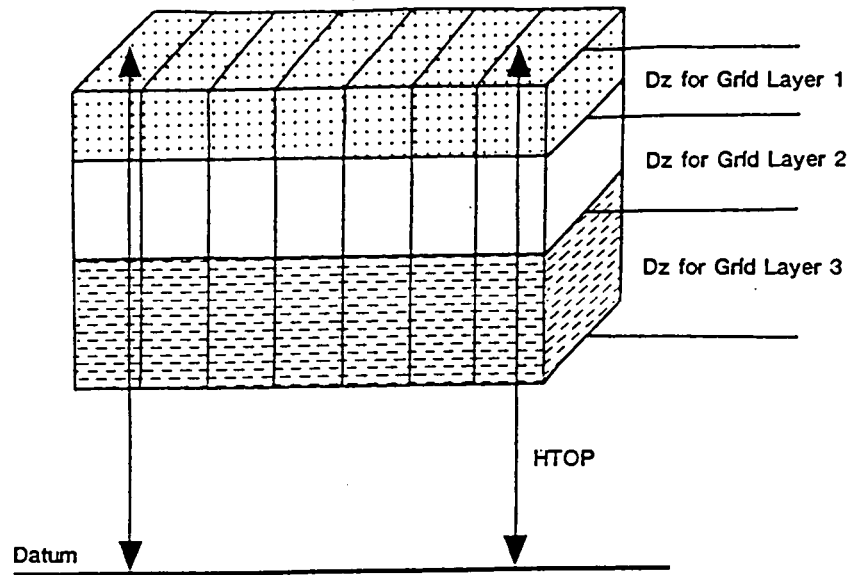
(a) Horizontal layers
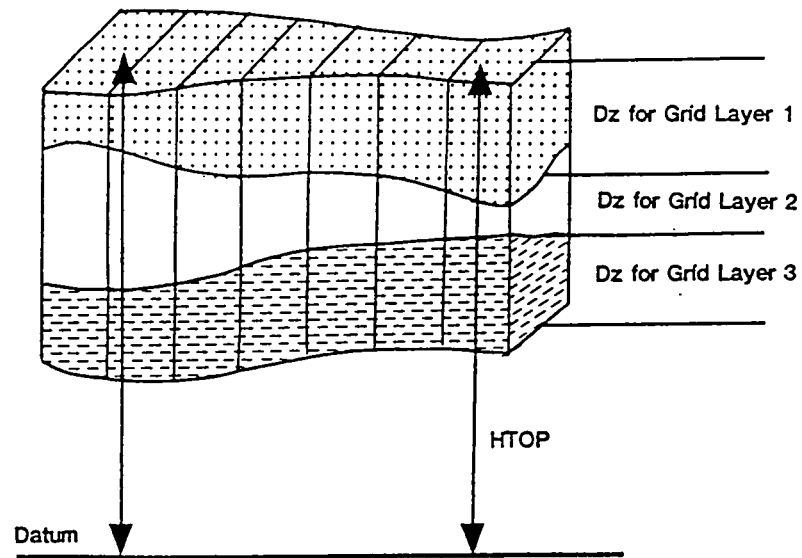
(b) Distorted layers

Fig. 6.3. 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).

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 will 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, $0.5 \leq PERCEL \leq 1$. 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 MIXELM=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, the first-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 if 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=0, 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>0, 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 grid (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, $0 \leq NPMIN \leq 4$ 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 NPMAX 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≥1). 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: 3I10

- INTERP is a flag indicating the concentration interpolation method for use in the MMOC solution scheme. Currently, only linear interpolation is implemented. Enter INTERP=1.

- 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 MIXELM=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.
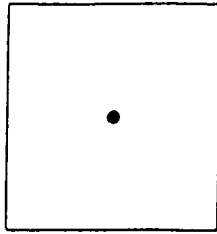
Fixed pattern 1:
Particle number per plane   1
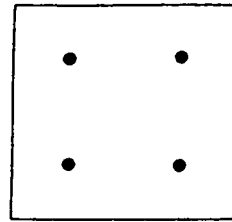
Fixed pattern 2:
Particle number per plane   4
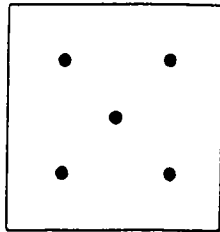
Fixed pattern 3:
Particle number per plane   5
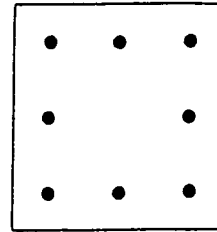
Fixed pattern 4:
Particle number per plane   8
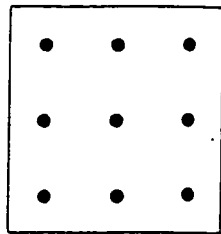
Fixed pattern 5:
Particle number per plane   9
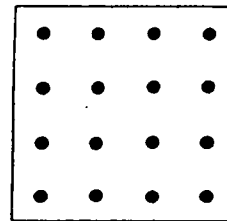
Fixed pattern 6:
Particle number per plane   16

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.

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 (α_L) for each cell in the grid. (Unit: L).

C2   Array: TRPT(NLAY)
       Reader: RARRAY
- TRPT is the ratio of the horizontal transverse dispersivity (α_{TH}) to the longitudinal dispersivity (α_L). One value is specified for each layer.

C3   Array: TRPV(NLAY)
       Reader: RARRAY
- TRPV is the ratio of the vertical transverse dispersivity (α_{TV}) to the longitudinal dispersivity (α_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:

D1   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 flux will be read for the current stress period.

    If INCRCH$\geq$0, an array containing the concentration of recharge flux will be read.

               <0, the concentration of recharge flux will be reused from the last stress period. If INCRCH<0 is entered for the first stress period, the concentration of recharge flux is set to zero by default.

(Enter D4 if FRCH=T <u>and</u> 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 specified 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$\geq$0, an 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 <u>and</u> 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 unformatted 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>0)

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. ITYPE 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.

6.9 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=1, 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>0)
E3 Array: SP1(NLAY)
    Reader: RARRAY

- SP1 is the first sorption constant. One value is specified each layer. The use of SP1 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_l). (Unit: L^3M^{-1}).

(Enter E4 if ISOTHM>0)

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 ($\bar{s}$). (Unit: MM^{-1}).

(Enter E5 if 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^{-1}). 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 of 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     Total 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.FIL) 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, type:

```
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 similar 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 file 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.

<div align="right">

Chapter 7

</div>

VERIFICATION AND APPLICATION

In this chapter, the accuracy of the MT3D 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:

$$C(x,0) = 0$$
$$C(0,t) = C_o \qquad t > 0$$
$$\frac{\partial C}{\partial x}(\infty,t) = 0 \qquad t > 0$$

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 (Δx) = 10 ft

Cell width along columns (Δy) = 1 ft

Layer thickness (Δz) = 1 ft

Groundwater seepage velocity (v) = 0.24 ft/day

Porosity (θ) = 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, α_L, retardation factor, R, and decay rate constant, λ as follows:

Case 1: $\alpha_L = 0$, $R = 0, \lambda = 0$.   Advection only.

Case 2: $\alpha_L = 10\,ft, R = 0, \lambda = 0$.   Advection and dispersion.

Case 3: $\alpha_L = 10\,ft, R = 5, \lambda = 0$.   Advection, dispersion and sorption.

Case 4: $\alpha_L = 10\,ft, R = 5, \lambda = 0.002\,day^{-1}$. 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-dimensional 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. 7.1a). Note that no numerical dispersion is introduced 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.
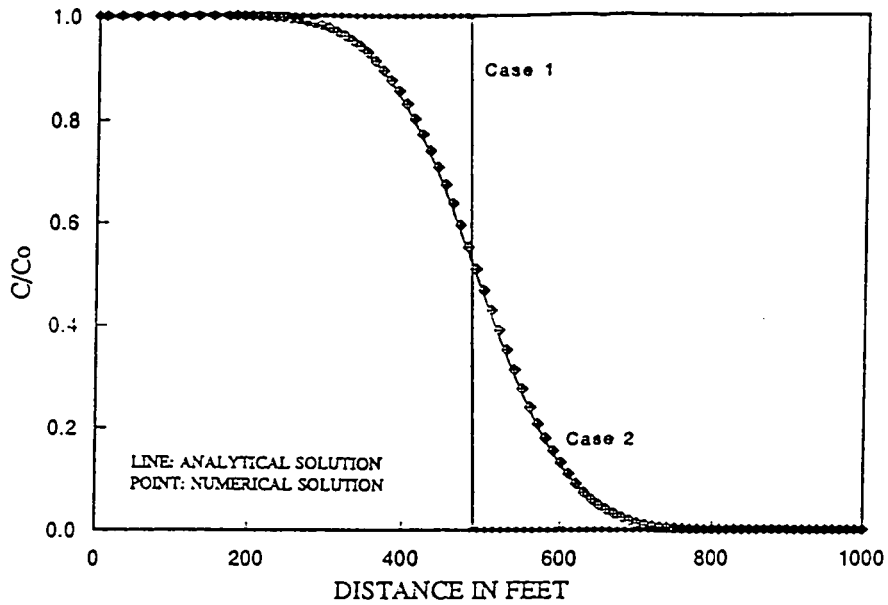
(a) Without sorption and decay
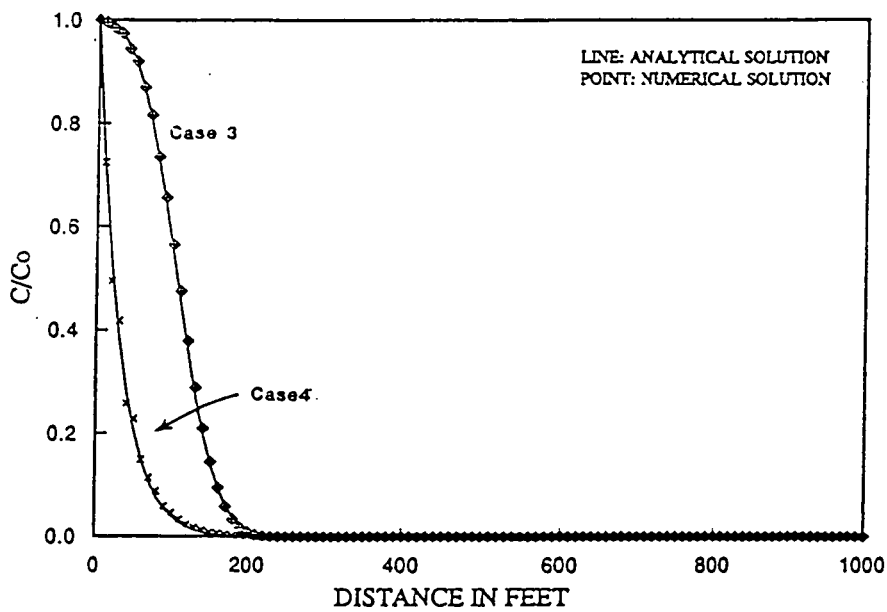
(b) With sorption and/or decay

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 Miller (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 (Δx) = 10 m

Cell width along columns (Δy) = 10 m

Layer thickness (Δz) = 10 m

Groundwater seepage velocity (v) = 1/3 m/day

Porosity (θ) = 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=1, 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=1) 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=1). 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.
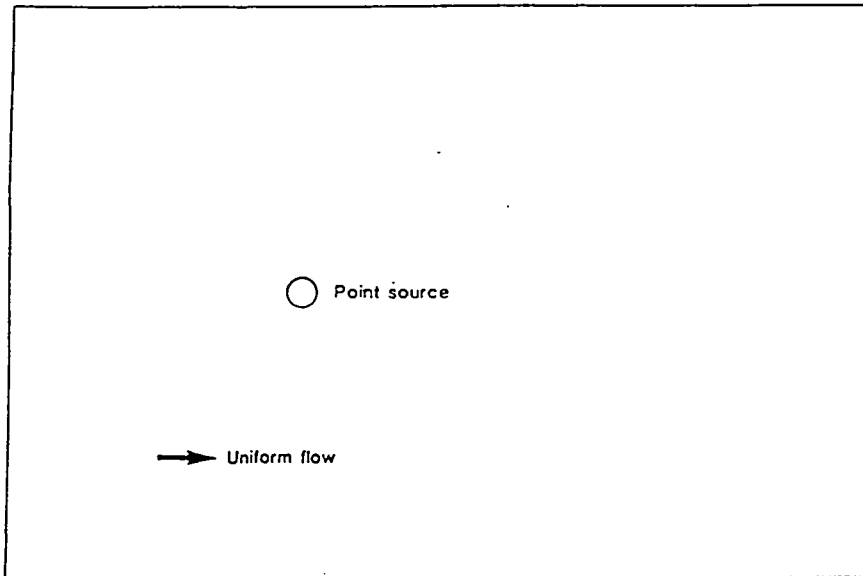
(a) Configuration of the flow field
simulated in the test problem
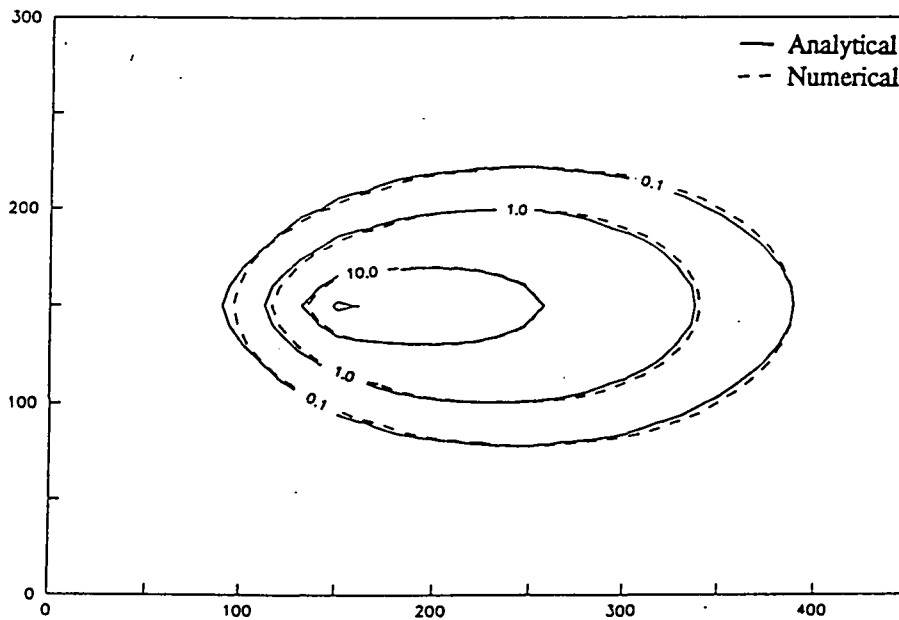
(b) Concentration plume as calculated by
the analytical and numerical solutions

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

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

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

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 (Δx) = 10 ft

Cell width along columns (Δy) = 10 ft

Layer thickness (Δz) = 1 ft

Porosity (θ) = 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 MMOC scheme):

INTERP=1, NLSINK=1,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 NPMAX 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.
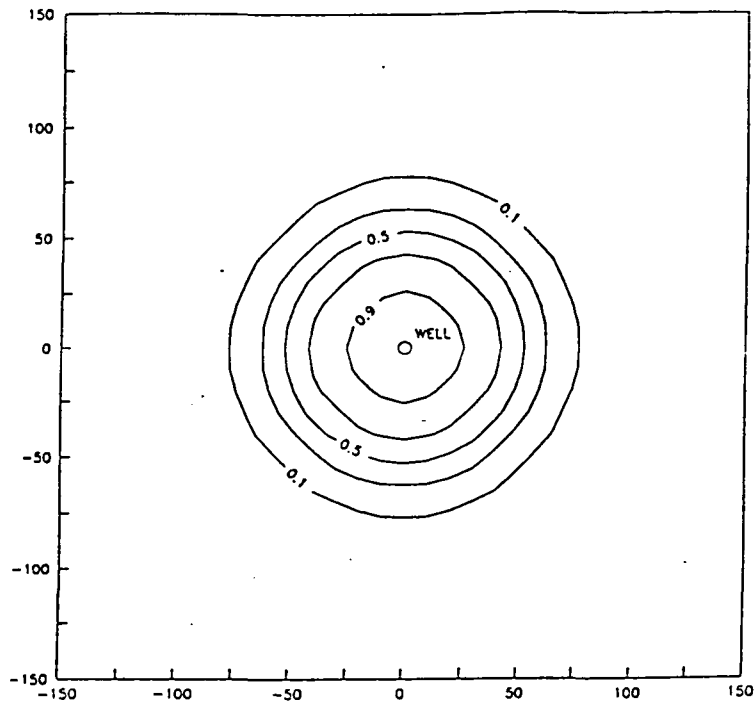
(a) Contour map of the concentration field
as calculated by the MT3D model
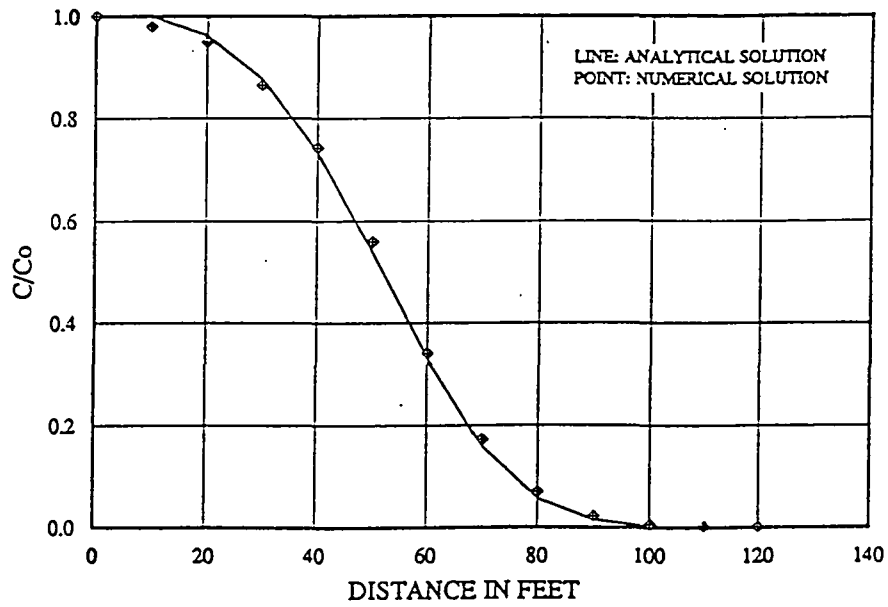
(b) Breakthrough curve along the X axis

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

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_o) 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 (Δx) = 900 ft

Cell width along columns (Δy) = 900 ft

Layer thickness (Δz)= 20 ft

Hydraulic conductivity of the aquifer = 0.005 ft/s
Porosity (θ) = 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 randomly 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:
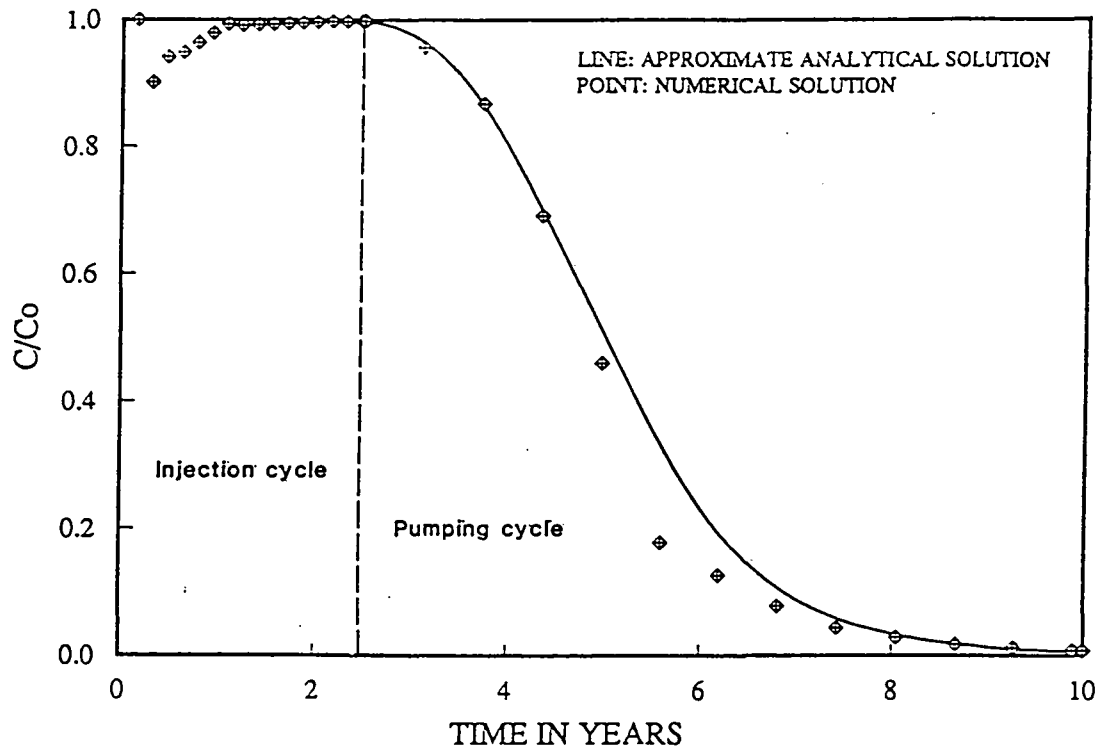
Fig. 7.4. Concentration at the well during an injection/pumping cycle as calculated by the MT3D model and the analytical solution in a strongly diverging/converging flow field.

Cell width along rows (Δx) = 10 ft

Cell width along columns (Δy) = 10 ft

Layer thickness (Δz) = 10 ft

Groundwater seepage velocity = 0.5 ft/day

Porosity (θ) = 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.
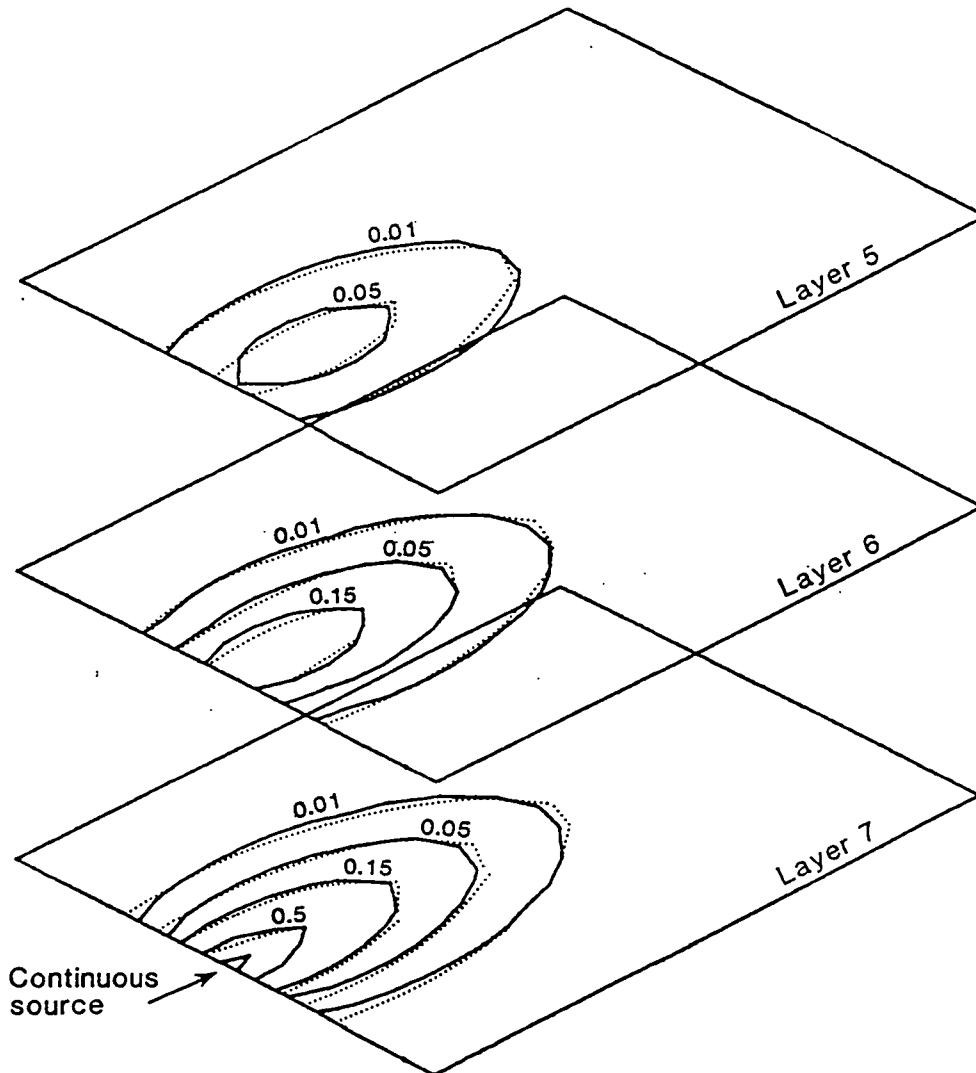
Fig. 7.5. Comparison of the numerical and analytical solutions for three-dimensional transport from a point source in a uniform flow field.

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 (Δx) = 100 m

Cell width along columns (Δy) = 100 m

Layer thickness (Δz) = 10 m

Porosity (θ) = 0.3

Longitudinal dispersivity = 20 ft

Ratio of horizontal transverse to longitudinal dispersivity = 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.

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
$= 1.474 \times 10^{-7} m / s$

Aquifer thickness
= 10m

Low K zone

Hydraulic conductivity
$= 1.474 \times 10^{-4} m / s$

PUMPING WELL

$Q = -0.0189 \, m^3 / s$

Y=1800m

No-mass flux boundary (transport model) No-flow boundary (flow model)

No-mass flux boundary (transport model) No-flow boundary (flow model)

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.

The HMOC option was used in the transport simulation with DCHMOC set equal to 2×10^{-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):

INTERP=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.

The 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.
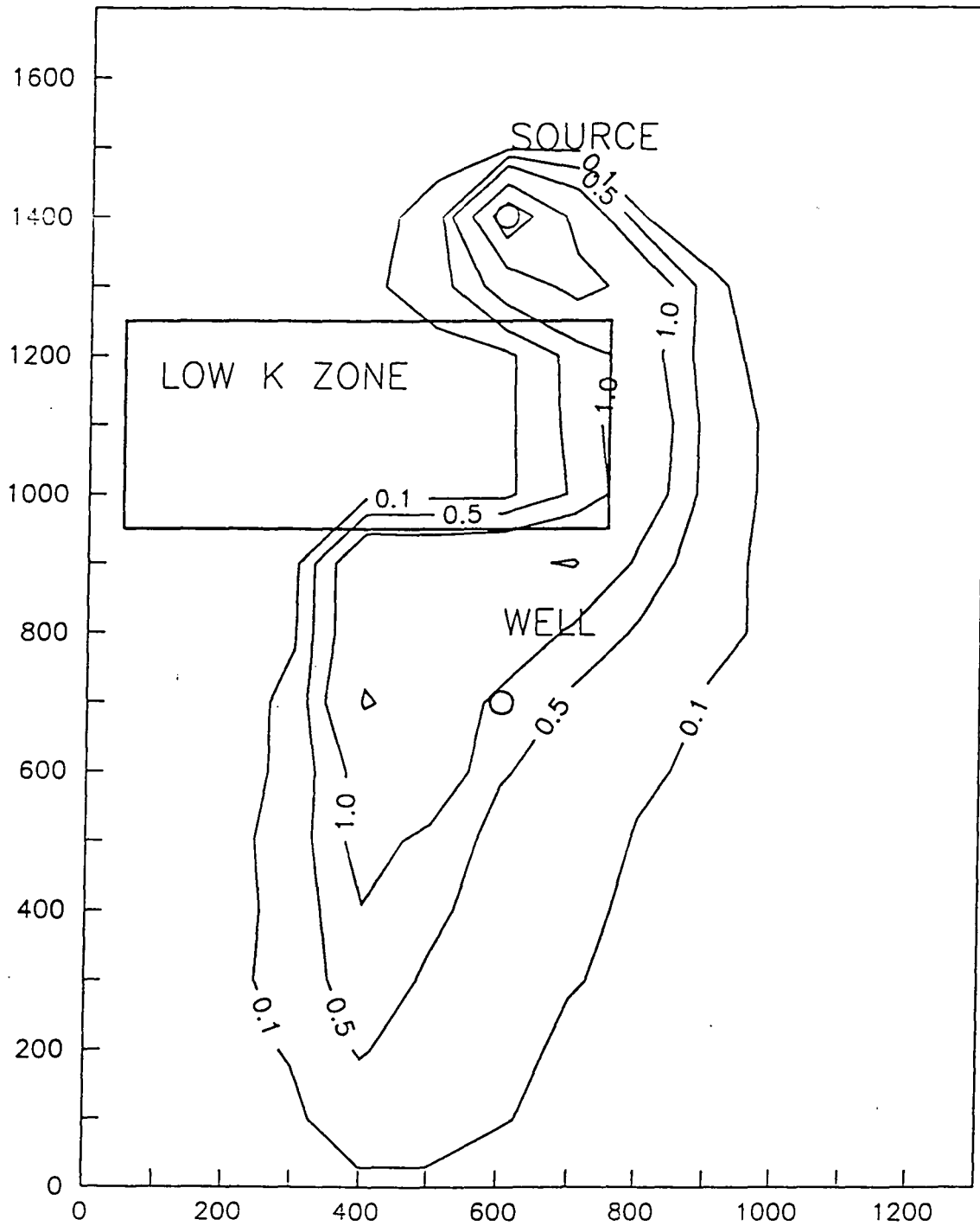
Fig. 7.7. Distribution of solute concentrations as solved by the hybrid MOC/MMOC (HMOC) solution.
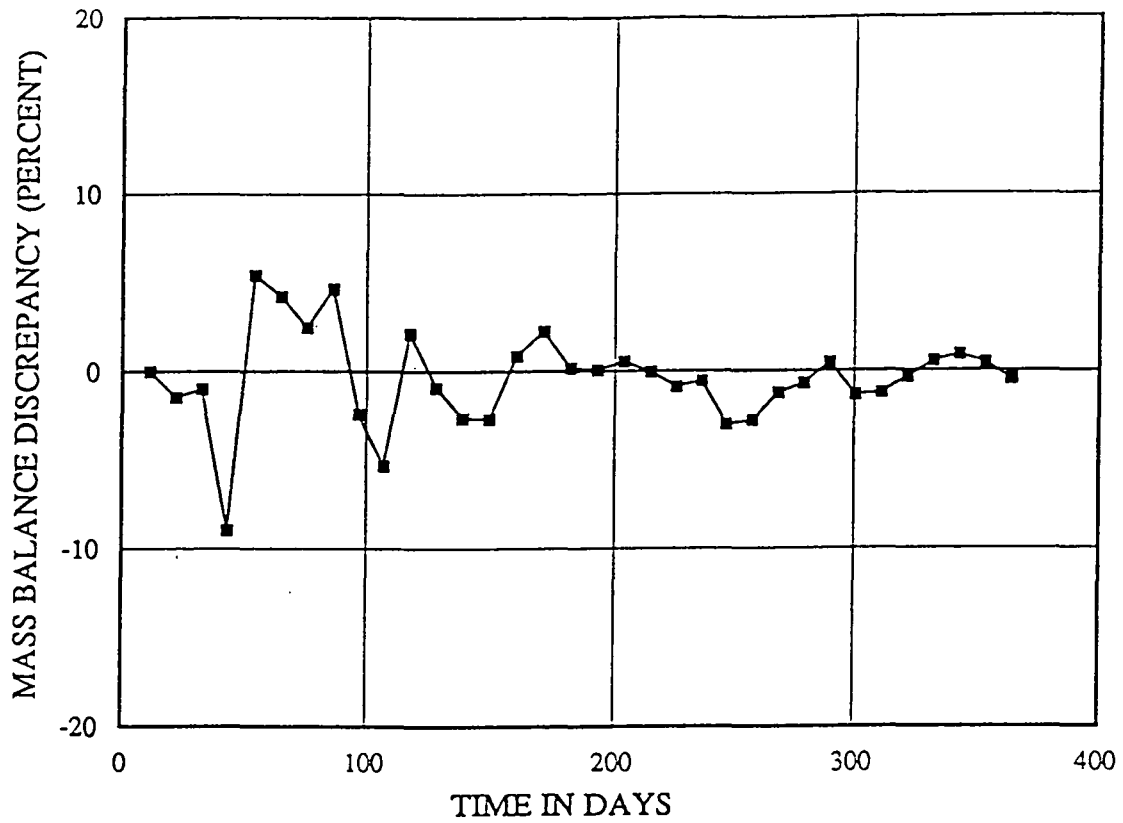
Fig. 7.8. Plot of the mass balance discrepancy error at each transport step for the test problem involving a heterogeneous aquifer.
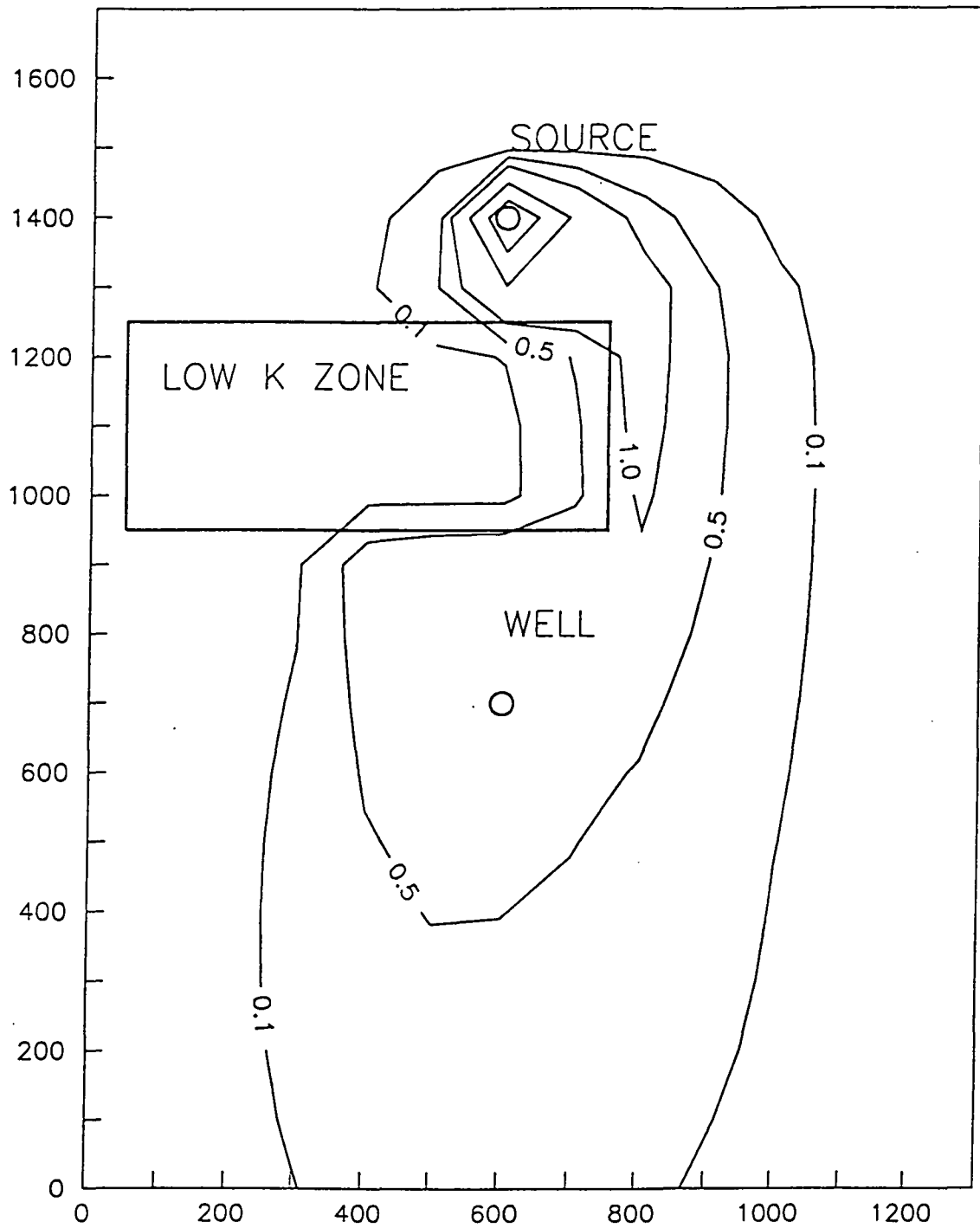
Fig. 7.9. Distribution of solute concentrations as solved by the finite difference solution for comparison with those solved by the hybrid MOC/MMOC (HMOC)solution (Fig. 7.7).

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 cells 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 W1 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 HMOC 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, NPMAX=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) was entered 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 W1, 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.
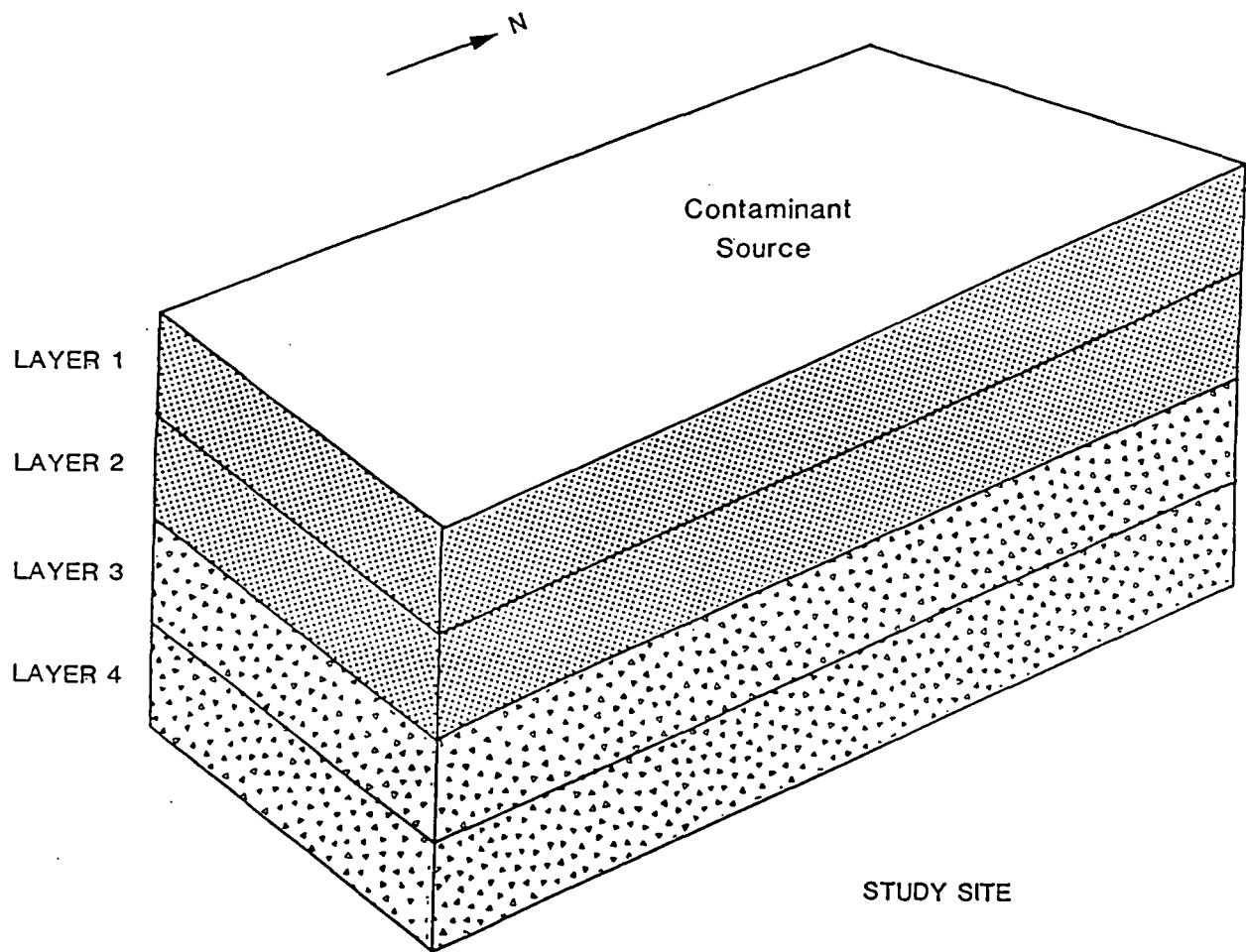
Fig. 7.10. Setting and vertical discretization in the field example.
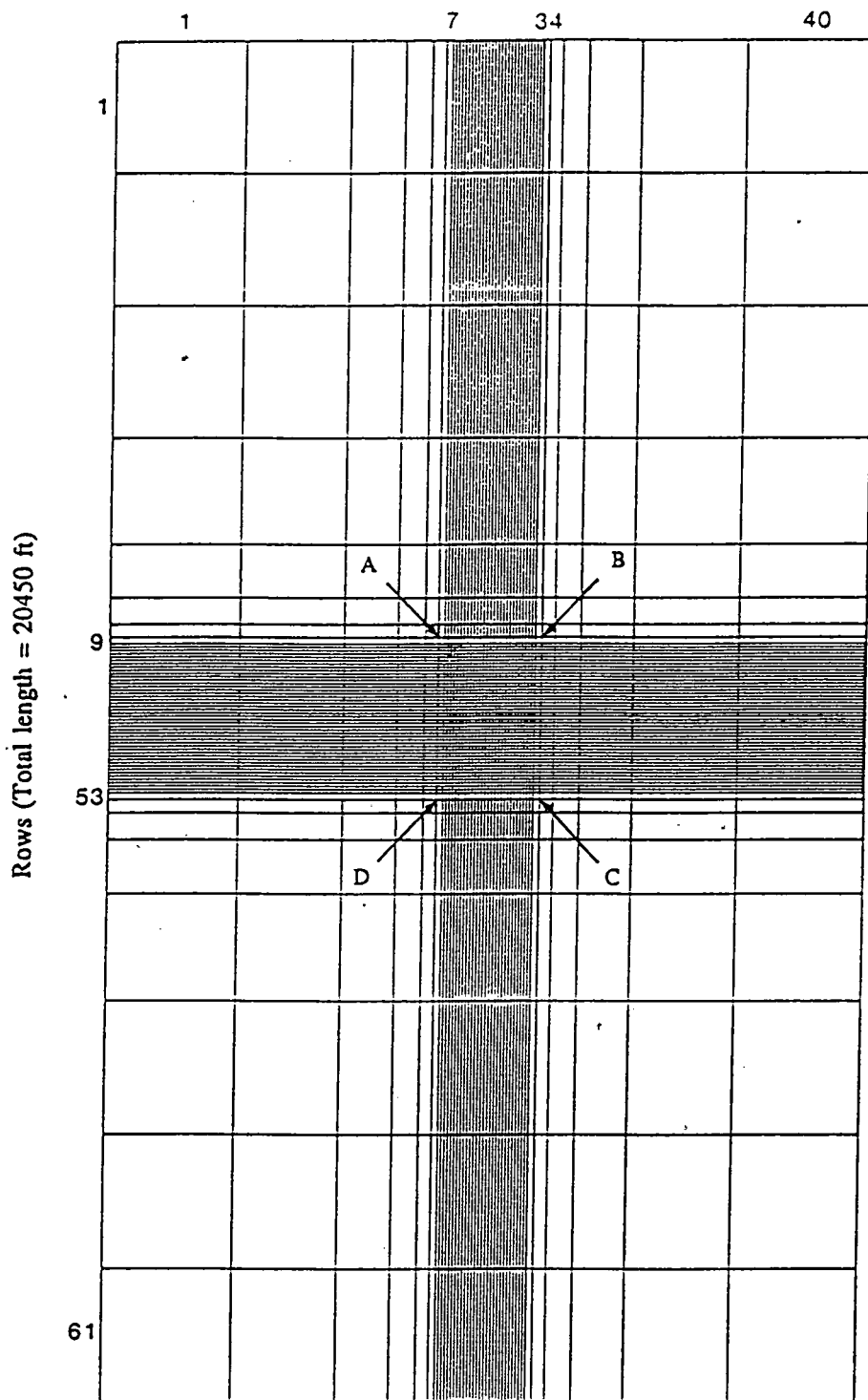
Fig. 7.11. Plan view of the finite difference mesh for the field example.
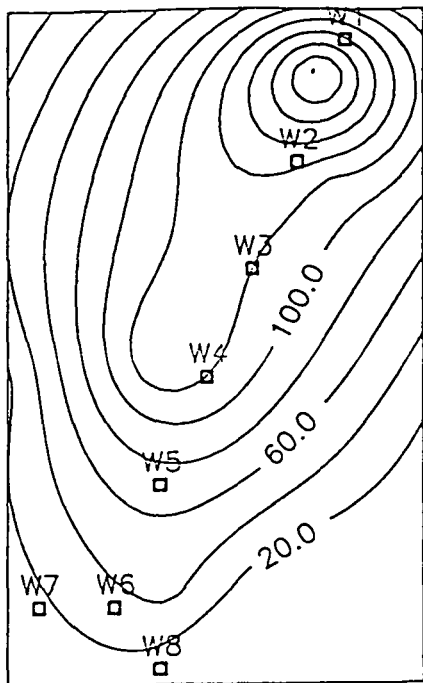
(a) Time=0 Days
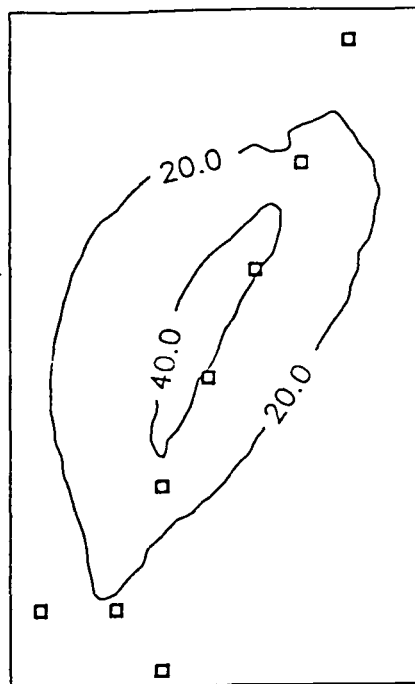
(b) Time=500 Days
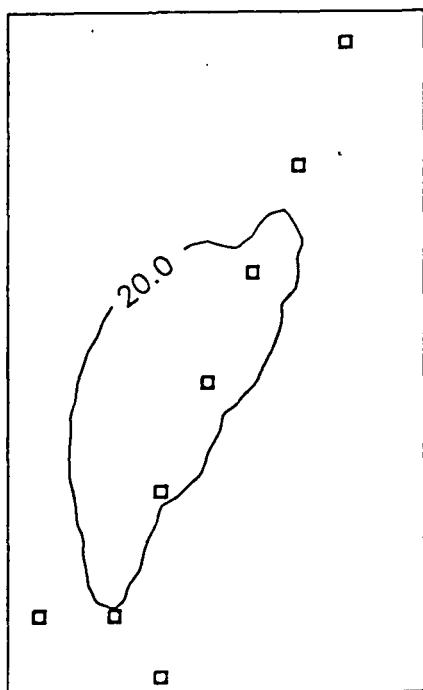
(c) Time=750 Days
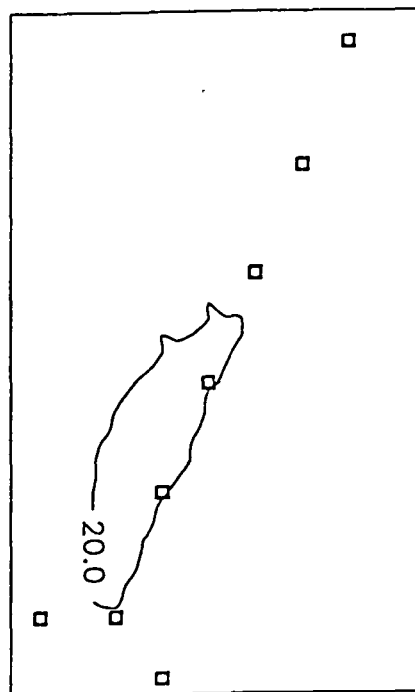
(d) Time=1000 Days

Fig. 7.12. Present distribution of the disolved 1,2-DCA and the model-predicted concentration changes at selected times after pumping starts
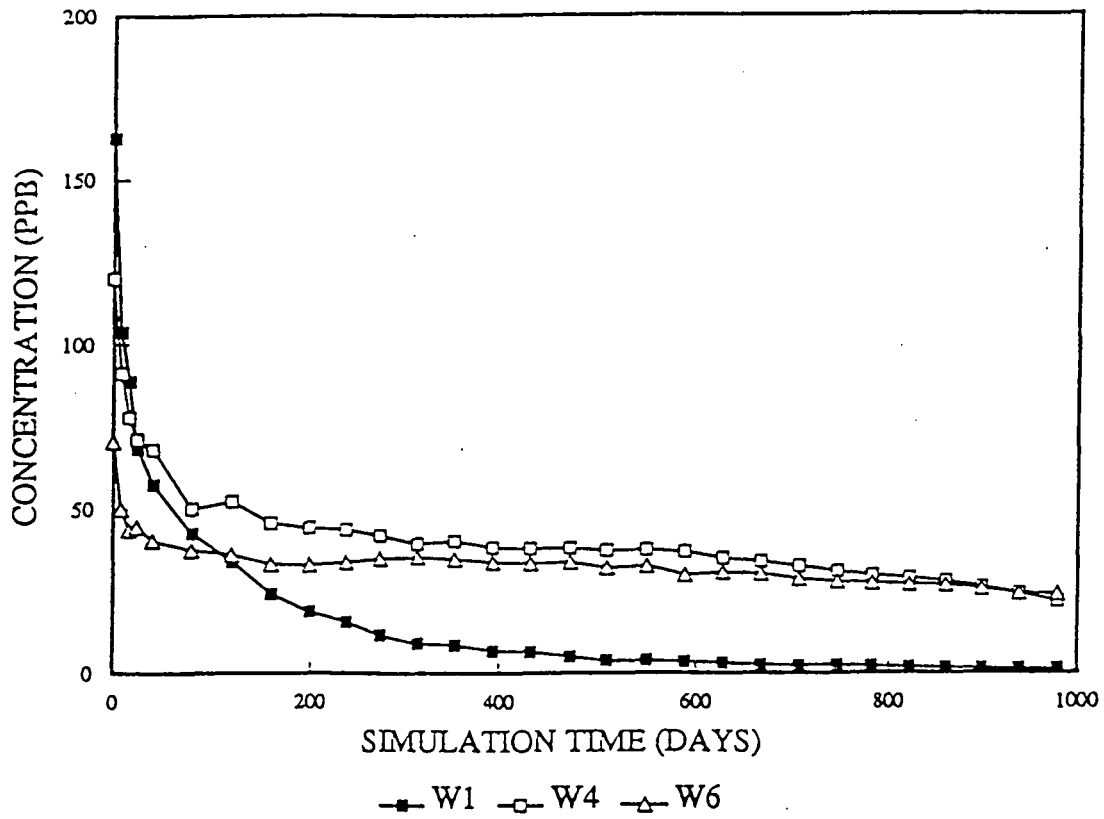
Fig. 7.13. Concentration breakthrough curves at pumping wells W1, W4 and W6, located at the northern end, middle area and southern end of the plume, respectively. (Concentrations are shown in the plot every five steps.)

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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 maximum 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=1 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

$(ND+1)*MXPART$

II. IX Array

$NODES$

C. DISPERSION PACKAGE (DSP)

I. X Array

$(ND^2+1)*NODES+3*NLAY$

II. IX 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

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:
    F1.   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 1.E30.
               LABEL='HEAD', identifying character label for heads
    (If NCOL=1, 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 NWEL>0, there must be NWEL 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           |NLAY,NROW,NCOL
DAY FT  UNDF                                        |LUNIT,TUNIT,MUNIT
T T T T                                            |ADV,DSP,SSM,RCT
   1 0 0 0 0 0                                      |LAYCON
         103        0.                         7   |ARRAY CONTROL-RECORD FOR DELR
2000.00 1600.00  800.00  400.00  200.00  100.00
28*50
100.00   200.00  400.00  800.00  1600.0 2000.00
         103        0.                         7   |DELR ENTERED IN FREE FORM
                                                   |ARRAY CONTROL-RECORD FOR DELC
2000.00 2000.00 2000.00 1600.00  800.00
400.00   200.00  100.00 45*50 100.00   200.00
400.00   800.00 1600.00 2000.00 2000.00 2000.00   |DELC ENTERED IN FREE FORM
         0       780.                              |HTOP, ENTERED AS A UNIFORM VALUE
         0        25.00                            |DZ-LAYER1, ENTERED AS A UNIFORM VALUE
         0        25.00                            |DZ-LAYER2
         0        25.00                            |DZ-LAYER3
        ·0        25.00                            |DZ-LAYER4
         0         .30                             |POROSITY-LAYER1
         0         .30                             |POROSITY-LAYER2
         0         .30                             |POROSITY-LAYER3
         0         .30                             |POROSITY-LAYER4
         0         1                               |ICBUND-LAYER1
         0         1                               |ICBUND-LAYER2
         0         1                               |ICBUND-LAYER3
         0         1                               |ICBUND-LAYER4
         0        0.                               |SCONC-LAYER1
        99       .2(20F8.3)                     5   |SCONC-LAYER2 (READ FROM EXTERNAL FILE ON UNIT 99)
        99       1.(20F8.3)                     5   |SCONC-LAYER3 (READ FROM EXTERNAL FILE ON UNIT 99)
         0        0.                               |SCONC-LAYER4
   -999.99                                         |CINACT
         8         2         0         0     T     |IFMTCN,IFMTNP,IFMTRF,IFMTDP,SAVUCN
         1                                         |NPRS
       500                                         |TIMPRS
         8                                         |NOBS
         3        11        29                     |KOBS,IOBS,JOBS
         3        19        26
         3        26        23
         3        33        20
         3        40        17
         3        48        14
         3        48         9
         3        52        17
         T                                         |CHKMAS
      1000.         1        1.                    |PERLEN,NSTP,TSMULT
        0.       1000                              |DTO,MXSTRN
```

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


INPUT FILE TO DSP PACKAGE
--------------------------
        0        10.                                             |AL-LAYER1, ENTERED AS A UNIFORM VALUE
        0        10.                                             |AL-LAYER3
        0        10.                                             |AL-LAYER3
        0        10.                                             |AL-LAYER4
        0        .20                                             |TRPT, ENTERED AS A UNIROM VALUE
        0        .20                                             |TRPV
        0        0.                                              |DMCOEF


INPUT FILE TO SSM PACKAGE
--------------------------
   T F T F F F                                                   |FWEL,FDRN,FRCH,FEVT,FRIV,FGHB
     2000                                                        |MXSS
        1                                                        |INCRCH
        0         0.                                             |CRCH, ENTERED AS A UNIFORM VALUE
        0                                                        |NSS


INPUT FILE TO RCT PACKAGE
--------------------------
        1         0                                             |ISOTHM,IREACT
        0        .3                                             |RHOB, ENTERED AS A UNIFORM VALUE
        0        1.                                             |SP1
        0        1.                                             |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 TRANSPORT MODEL FOR REMEDIAL DESIGN
 | 3 D | (REFER TO SECTION 7.7)
  -----

THE TRANSPORT MODEL CONSISTS OF    4 LAYER(S)   61 ROW(S)   40 COLUMN(S)
NUMBER OF STRESS PERIOD(S) IN SIMULATION =    1
UNIT FOR TIME IS DAY ;  UNIT FOR LENGTH IS FT  ;  UNIT FOR MASS IS UNDF
MAJOR TRANSPORT COMPONENTS TO BE SIMULATED:
 1  ADVECTION
 2  DISPERSION
 3  SINK AND SOURCE MIXING
 4  CHEMICAL REACTIONS (DECAY AND/OR SORPTION)

BTN1 -- BASIC TRANSPORT 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 FROM UNIT  2
ADVECTION IS SOLVED WITH THE HYBRID [MOC]/[MMOC] SCHEME
COURANT NUMBER ALLOWED IN SOLVING THE ADVECTION TERM =  1.00
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 1.0, 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
TYPE 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

OUTPUT CONTROL OPTIONS

PRINT CELL CONCENTRATION USING FORMAT CODE: 8
PRINT PARTICLE NUMBER IN EACH CELL USING FORMAT CODE: 2
PRINT RETARDATION FACTOR USING FORMAT CODE: 0
DO NOT PRINT DISPERSION COEFFICIENT
SAVE CONCENTRATION IN UNFORMATTED FILE [MT3D.UCN] ON UNIT 18

NUMBER OF TIMES AT WHICH SIMULATION RESULTS 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 SUMMARY 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 =   0.500
THE CONCENTRATION GRADIENT 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 "MMOC" 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) =   10.00000   FOR LAYER 3
                                    LONG. DISPERSIVITY (AL) =   10.00000   FOR LAYER 4
                                    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-SPECIFIED TRANSPORT STEPSIZE = 0.0000000   DAY
MAXIMUM NUMBER OF TRANSPORT STEPS 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.F.=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 SOURCES/SINKS PRESENT IN THE FLOW MODEL =   800

MAXIMUM STEPSIZE WHICH MEETS STABILITY CRITERION OF THE SINK & SOURCE TERM
= 553.2   (WHEN MIN. 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.=1) 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
PARTICLES 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

       PARTICLE NUMBER IN LAYER 3 AT END OF TRANSPORT STEP   64, TIME STEP 1, STRESS PERIOD 1

       PARTICLE NUMBER IN LAYER 4 AT END OF TRANSPORT STEP   64, TIME STEP 1, STRESS PERIOD 1

       CUMMULATIVE 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 SINCE BEGINNING OF SIMULATION =   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, 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
      0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   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  0.3  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  0.1  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  0.0
 6   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  0.1  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  0.2  0.0  0.0  0.0
     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  0.6  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  0.4  0.5  0.5  0.5  0.7  0.6  0.8  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  0.3
     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  0.3  0.4  0.4  0.6  0.6  0.7  0.8  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  1.5  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  5.2  5.4  5.8  5.8  0.0
     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  0.4  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  0.0
    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  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
    15.4 14.0 14.0 11.2  9.5  8.0  6.8  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
35   0.0  0.0  0.0  0.1  1.3  4.4  6.5  7.9 10.3 12.5 15.0 17.0 19.2 21.2 23.2 25.9 27.4 28.5 21.4 15.8
    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 23.2 25.9 27.4 28.5 21.4 15.8  0.0
    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  5  8  9  6  7  0  0  0  0  0  0  0  0
 6    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  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  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
 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  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  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  9 10 15  9 10 11 12  5  5  7  3  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  4 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 12  6  9  7  5  6  3  5  6  7  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
33  0  0  0 14 13 14  6 15 13 18 12  9  5  6 13  3  5  8  5 19 11  9 15 11  8 13  6 10 12 13  7  9  6  5  6  4  7  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
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
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
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
38  0  0  0 13  7  5  8  7  8  9 12  9 11 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
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  9  9 10  5  5  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
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
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
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
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 14 11 11 11 10  7 15  4  1  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 11 10  3 10  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 13  6  3  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 18  9  2 10  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
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
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
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
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
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
54  0  0  0  0  0  0  8 16 20 17 16 12  7  4 10  9  9  9  9 10  0  0
55  0  0  0  0  0  0 10 24 23 26  8 10 16  5 13 15  6  0  0
56  0  0  0  0  0  0  4 23 10 12 11 15  3  0  0
57  0  0  0  0  0  0  0  0  0  0  1  0  0
58  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
60  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
```

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

CUMMULATIVE 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
WELLS:	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	-0.1835388E+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

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 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, 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 equal to T. The structures and contents of these two files are as follows:

MT3D.UCN (saved unformatted):

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=1,NCOL),I=1,NROW)

where

NTRANS	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 time 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;

| ILAY | 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, NCOL
Record 2:	(DELR(J), J=1,NCOL)
Record 3:	(DELC(I),I=1,NROW)
Record 4:	((HTOP(J,I), J=1,NCOL),I=1,NROW)
Record 5:	(((DZ(J,I,K), J=1,NCOL),I=1,NROW),K=1,NLAY)
Record 6:	CINACT

where

NLAY	is the total number of layers;
DELR	is the cell width along the row direction;
DELC	is the cell width along the column direction;
HTOP	is the top elevation of the first model layer;
DZ	is the thickness of each cell in the grid; and
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, whichever is more convenient. The user can also define a "window" within which the graphic data files are desired by specifying the *starting* and *ending* column (J), row (I) and layer (K) indices 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 starting (J, I, K) indices as 5, 20, 1, and the ending (J, I, K) indices 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 starting (J, I, K) indices as 20, 5, 1, and the ending indices 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 starting (J, I, K) indices 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 starting (J, I, K) indices as 20, 1, 0 and the ending indices as 40, 10, 0.

It should be pointed out that in the MT3D model, the origin of the coordinate system is set at the upper, top, left corner of cell (1, 1, 1) and the positive x, y and z coordinates are in the directions of increasing column, row, and layer indices, respectively (see Fig. D-1). However, in the output files generated by POSTMT3D, the origin is transformed to the lower, bottom, right corner of cell (1, NROW, NLAY), as is customary in most graphic programs. As a result, the y and z axes used in MT3D are reversed by POSTMT3D whereas the x axis remains the same (see Fig. D-1).

Therefore, if the contour map is on a layer or water table (i.e., the x-y plane), the horizontal axis of the map is along the direction of increasing column (J) indices, and the vertical axis is along the direction of decreasing row (I) indices. If the contour map is on a cross section along a row (i.e., the x-z plane), the horizontal axis of the map is along the direction of increasing column (J) indices, and the vertical axis is along the direction of decreasing layer (K) indices. If the contour map is on a cross section along a column (i.e., the y-z plane), the horizontal axis of the map is along the direction of decreasing (I) indices, and the vertical axis is along the direction of decreasing layer (K) indices. All the necessary transformations are done by POSTMT3D automatically.

Cell (1,1,1)
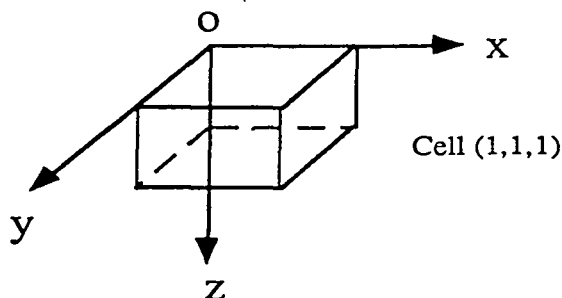
(a) The coordinate system used in MT3D

Cell (1, NROW, NLAY)
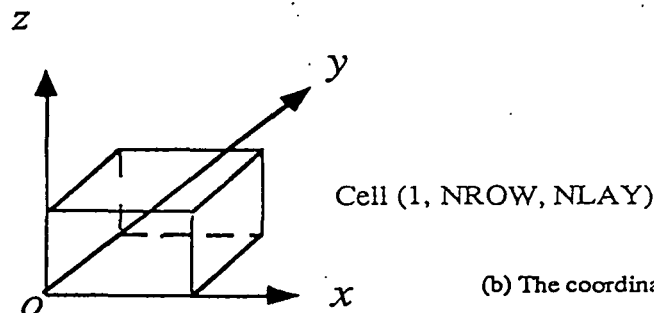
(b) The coordinate system used in POSTMT3D

Fig. D-1. Transformation of coordinates from MT3D to POSTMT3D

For output, POSTMT3D writes data files in one of the two formats, referred to as the
".GRD" format and the ".DAT" format, according to the convention used by Golden Software's
SURFER® graphic package. The .GRD 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 and SURF programs
included in SURFER®. The .DAT format as listed below writes the concentration at each node
with the nodal coordinates within the user-defined 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 concentrations versus distances along a column, row or layer at at
a selected time. (Note that the plots of concentrations versus times at a selected node can be
generated from the observation point file, MT3D.OBS, saved by MT3D.)

.GRD file format (saved in free format):

DSAA

NX, NY, XMIN, XMAX, YMIN, YMAX, CMIN, CMAX

((CWIN(JJ,II),JJ=1,NX),II=NY,1,-1)

where

DSAA	is the character string identifying the .GRD format;
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.

.DAT file format (saved in free format):

For each active cell:

    X, Y, CXY

where

APPENDIX B

MODEL INPUT

APPENDIX B.1

FLOW MODEL INPUT

NODE		HEAD	S+G BOT. or BR BOT.	S+G SAT. THK.	BDRK SAT. THK.	0.000416 S+G T	0.000083 BDRK T	COMPOSITE T ft^2/sec	COMPOSITE K ft/sec
X	Y								
851	50	907.5	col 1 658	247.3	247.3	0.102876	0.0206	0.0206	0.000083
851	150	907.3	658	247.1	247.1	0.102793	0.020583	0.020583	0.000083
851	250	907.1	658	246.9	246.9	0.10271	0.020566	0.020566	0.000083
851	350	906.9	658	246.7	246.7	0.102627	0.02055	0.02055	0.000083
851	450	906.7	658	246.5	246.5	0.102544	0.020533	0.020533	0.000083
851	550	906.5	658	246.3	246.3	0.10246	0.020516	0.020516	0.000083
851	650	906.3	658	246.1	246.1	0.102377	0.0205	0.0205	0.000083
851	750	906.1	658	245.9	245.9	0.102294	0.020483	0.020483	0.000083
851	850	905.9	658	245.7	245.7	0.102211	0.020466	0.020466	0.000083
851	950	905.7	658	249.5	249.5	0.103792	0.020783	0.020783	0.000083
851	1050	905.5	658	249.3	249.3	0.103708	0.020766	0.020766	0.000083
851	1150	905.3	658	249.1	249.1	0.103625	0.02075	0.02075	0.000083
851	1250	905.1	658	248.9	248.9	0.103542	0.020733	0.020733	0.000083
851	1350	904.9	658	248.7	248.7	0.103459	0.020716	0.020716	0.000083
851	1450	904.7	658	248.5	248.5	0.103376	0.0207	0.0207	0.000083
851	1550	904.5	658	248.3	248.3	0.103292	0.020683	0.020683	0.000083
851	1650	904.3	658	248.1	248.1	0.103209	0.020666	0.020666	0.000083
851	1750	904.1	658	247.9	247.9	0.103126	0.02065	0.02065	0.000083
851	1850	903.9	658	247.7	247.7	0.103043	0.020633	0.020633	0.000083
851	1950	903.7	658	247.5	247.5	0.10296	0.020616	0.020616	0.000083
2269.5	50	907.5	col 2 658	249.5	249.5	0.103792	0.020783	0.020783	0.000083
2269.5	150	907.3	658	249.3	249.3	0.103708	0.020766	0.020766	0.000083
2269.5	250	907.1	658	249.1	249.1	0.103625	0.02075	0.02075	0.000083
2269.5	350	906.9	658	248.9	248.9	0.103542	0.020733	0.020733	0.000083
2269.5	450	906.7	658	248.7	248.7	0.103459	0.020716	0.020716	0.000083
2269.5	550	906.5	658	248.5	248.5	0.103376	0.0207	0.0207	0.000083
2269.5	650	906.3	658	248.3	248.3	0.103292	0.020683	0.020683	0.000083
2269.5	750	906.1	658	248.1	248.1	0.103209	0.020666	0.020666	0.000083
2269.5	850	905.9	658	247.9	247.9	0.103126	0.02065	0.02065	0.000083
2269.5	950	905.7	658	247.7	247.7	0.103043	0.020633	0.020633	0.000083
2269.5	1050	905.5	658	247.5	247.5	0.10296	0.020616	0.020616	0.000083
2269.5	1150	905.3	658	247.3	247.3	0.102876	0.0206	0.0206	0.000083
2269.5	1250	905.1	658	247.1	247.1	0.102793	0.020583	0.020583	0.000083
2269.5	1350	904.9	658	246.9	246.9	0.10271	0.020566	0.020566	0.000083
2269.5	1450	904.7	658	246.7	246.7	0.102627	0.02055	0.02055	0.000083
2269.5	1550	904.5	658	246.5	246.5	0.102544	0.020533	0.020533	0.000083
2269.5	1650	904.3	658	246.3	246.3	0.10246	0.020516	0.020516	0.000083
2269.5	1750	904.1	658	246.1	246.1	0.102377	0.0205	0.0205	0.000083
2269.5	1850	903.9	658	245.9	245.9	0.102294	0.020483	0.020483	0.000083
2269.5	1950	903.7	658	245.7	245.7	0.102211	0.020466	0.020466	0.000083
3215.5	50	907.5	col 3 840	67.5	182	0.02808	0.01516	0.02162	0.000086
3215.5	150	907.3	840	67.3	182	0.027996	0.01516	0.021578	0.000086
3215.5	250	907.1	840	67.1	182	0.027913	0.01516	0.021537	0.000086
3215.5	350	906.9	830	76.9	172	0.03199	0.014327	0.023159	0.000093
3215.5	450	906.6	830	76.6	172	0.031865	0.014327	0.023096	0.000092
3215.5	550	906.4	830	76.4	172	0.031782	0.014327	0.023055	0.000092
3215.5	650	906.2	830	76.2	172	0.031699	0.014327	0.023013	0.000092
3215.5	750	906	830	76	172	0.031616	0.014327	0.022971	0.000092
3215.5	850	905.8	830	75.8	172	0.031532	0.014327	0.02293	0.000092
3215.5	950	906.6	830	76.6	172	0.031865	0.014327	0.023096	0.000092
3215.5	1050	905.4	830	75.4	172	0.031366	0.014327	0.022847	0.000092
3215.5	1150	905.2	830	75.2	172	0.031283	0.014327	0.022805	0.000092
3215.5	1250	905	825	80	167	0.03328	0.013911	0.023595	0.000095
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3215.5	1450	904.6	820	84.6	162	0.035193	0.013494	0.024344	0.000098
3215.5	1550	904.5	820	84.5	162	0.035152	0.013494	0.024323	0.000098
3215.5	1650	904.3	830	74.3	172	0.030908	0.014327	0.022618	0.000091
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3215.5	1850	903.9	658	245.9	245.9	0.102294	0.020483	0.020483	0.000083
3215.5	1950	903.7	658	245.7	245.7	0.102211	0.020466	0.020466	0.000083

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INPUT DATA FOR BASIC PACKAGE

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BCF,RECHARGE,SIP,OCI-STEADY STATE
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               0   1
               1   1   (25I2)   -1
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903.9 903.9 903.9 903.9 903.9 903.9 904.0 904.1 904.2 904.2 904.3
904.4 904.5 904.6 904.7 904.8 904.8 904.9 905.0 905.1 905.1 905.2
905.2 905.3 905.4 905.4 905.5 905.5 905.5 905.6 905.6 905.7 905.8
905.9 906.1 906.3 906.5 906.7 906.9
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INPUT DATA FOR BLOCK-CENTERED FLOW PACKAGE

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 1702.01135.0 757.0 505.0 337.0 225.0 150.0 100.0 100.0 100.0 100.0
  100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0
  100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0
  100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 150.0
  225.0 337.0 505.0 757.01135.01702.0
            11          1.    (11F6.1)
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  100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0
            11        .00001   (11F6.2)                    -1
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   8.33   8.33   8.33   8.33   8.33   8.33   8.33   8.33   8.33   4.65   8.65
  10.72  12.79  14.86  15.60  16.20  16.80  17.47  18.07  18.67  19.27  16.87
  14.80  11.74   9.02   8.33   8.33   8.33
   8.33   8.33   8.65   8.33   8.33   8.33   8.33   8.33   8.33   8.33   8.33
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   8.33   8.33   8.33   8.33   8.33   8.33   8.33   8.33   8.33   5.97   9.31
  11.32  13.32  15.32  16.26  16.86  17.13  17.80  18.40  19.00  19.60  17.20
  14.80  12.07   9.35   8.33   8.33   8.33
   8.33   8.33   8.64   8.33   8.33   8.33   8.33   8.33   8.33   8.33   8.33
   8.33   8.33   4.96   4.96   8.33   8.33   8.33   8.33   8.33   8.33   8.33
   8.33   8.33   8.33   8.33   8.33   8.33   8.33   8.33   4.96   9.30  11.31
  13.31  15.32  16.19  16.39  16.93  17.46  18.00  18.53  19.06  19.60  17.20
  14.13  11.74   9.34   8.33   8.33   8.33
   8.33   8.33   9.30   8.33   8.33   8.33   8.33   8.33   3.94   4.61   4.61
   4.95   4.95   6.62   5.28   8.33   8.33   8.33   8.33   8.33   8.33   8.33
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  13.31  15.65  16.19  16.39  16.92  17.46  17.99  18.53  19.06  19.60  17.20
  14.13  11.73   9.34   8.33   8.33   8.33
   8.33   8.33   9.29   8.33   8.33   8.33   8.33   3.93   6.14   6.47   6.81
   6.81   6.81   8.35   7.14   5.94   8.33   8.33   8.33   8.33   8.33   8.33
   8.33   8.33   8.33   8.33   8.33   8.33   8.33   4.94   9.30  11.30  13.31
  15.32  16.12  16.32  16.86  17.39  17.93  18.46  19.00  19.60  17.66  15.79
  13.19  11.26   9.33   8.33   8.33   8.33
   8.33   8.33   9.27   8.33   8.33   8.33   3.93   7.60   7.93   8.27   8.60
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   8.33   8.33   8.33   8.33   8.33   8.33   4.93   9.96  11.30  12.64  15.31
  16.18  16.25  16.72  17.19  17.66  18.13  18.59  19.06  19.60  17.66  15.46
  13.19  11.26   8.66   8.33   8.33   8.33
   8.33   8.33   9.26   8.33   8.33   3.92   6.86   9.46   9.46  10.13  10.47
  10.48  10.48  11.42  10.48   9.34   7.86   5.92   5.99   5.92   5.92   5.92
   5.93   5.93   5.93   5.93   5.60   5.60   9.95  11.29  12.63  14.31  16.05
  16.72  16.72  17.19  17.66  18.12  18.59  19.06  19.60  17.66  15.79  13.52
  11.25   8.98   7.99   8.33   8.33   8.33
   8.33   8.33   9.25   8.33   8.33   4.57   8.26  11.67  12.01  12.01  12.01
  12.02  12.02  12.75  12.02  11.08   9.80   9.94   9.94   9.94   9.94   9.94
   9.94   9.94   9.94   9.95   9.95   9.95  10.28  12.96  14.30  15.98  16.25
  16.92  17.19  17.59  17.99  18.39  18.79  19.19  19.60  17.66  15.78  13.51
  11.24   9.31   8.33   8.33   8.33   8.33
   8.33   8.33   9.24   8.33   8.33   5.90   9.59  13.48  13.48  13.48  13.48
  13.48  13.48  14.09  13.48  12.74  11.74  11.88  11.88  11.88  11.88  11.88
  11.88  11.88  11.88  11.89  11.89  11.89  11.89  14.37  15.44  16.91  16.91
  17.45  17.65  18.05  18.46  18.86  19.26  19.60  17.99  16.38  14.44  12.97
  10.90   8.64   8.33   8.33   8.33   8.33
   8.33   8.33   9.23   8.33   8.33   8.57  11.80  15.02  15.02  15.02  15.02
  15.02  15.02  15.49  15.02  14.48  13.75  13.82  13.82  13.82  13.82  13.82
  13.82  13.82  13.82  13.83  13.83  13.83  13.83  15.44  16.24  17.58  17.58
  17.99  18.12  18.46  18.79  19.19  19.59  17.99  16.65  14.98  13.64  12.97
  10.63   8.97   8.33   8.33   8.33   8.33
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10.83  8.96  8.33  8.33  8.33  8.33
 8.33  8.33  9.22  8.54  9.23 13.26 15.62 18.04 18.04 18.04 18.04
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10.49  8.62  8.33  8.33  8.33  8.33
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 9.29  7.95  8.33  8.33  8.33  8.33
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 8.95  8.33  8.33  8.33  8.33  8.33
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15.36 15.70 16.03 16.04 16.37 15.64 14.29 13.96 12.75 12.28 12.62
 8.61  8.33  8.33  8.33  8.33  8.33
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11.55 11.21 10.88 10.54  9.53  8.86  8.87  8.33  8.54  8.54 11.91
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13.07 13.08 13.75 14.09 14.42 13.82 13.62 13.35 12.68 12.28 12.28
 8.60  8.33  8.33  8.33  8.33  8.33
 8.33  8.33  9.16 14.91 18.91 16.34 13.22 12.89 12.55 11.87 11.20
10.86 10.86 10.53  9.52  8.85  8.33  8.33  8.33  8.33  8.33  8.20
 8.54  8.55  7.87  7.54  7.21  7.55  7.55  9.57  9.57 11.12 11.12
11.12 11.46 11.80 11.80 12.47 12.34 12.27 12.41 12.28 11.94 11.95
 8.60  8.33  8.33  8.33  8.33  8.33
 8.33  8.33  8.33 13.22 18.91 16.34 13.22 12.55 11.87 11.19 10.86
10.52  9.85  9.17  8.50  8.50  8.33  8.33  8.33  8.33  8.33  8.33
 8.33  8.33  8.33  8.33  8.33  8.33  7.54  7.88  7.88  8.23  8.23
 8.23  8.23  8.23  9.24 10.52 10.86 10.93 11.80 18.25 11.60 11.94
 8.93  8.33  8.33  8.33  8.33  8.33
 8.33  8.33  8.33 13.22 18.91 16.33 13.22 11.87 11.19 10.51 10.51
 9.50  9.16  8.33  8.33  8.33  8.33  8.33  8.33  8.33  8.33  8.33
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 8.33  8.33  7.89  7.90  8.57  9.71  9.92 11.19 11.06 10.93 11.27
 8.59  8.33  8.33  8.33  8.33  8.33
 8.33  8.33  8.33 13.22 18.91 16.33 13.22 11.60 10.72  9.84  9.16
 9.16  8.14  8.33  8.33  8.33  8.33  8.33  8.33  8.33  8.33  8.33
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 8.33  8.33  8.33  8.33  7.89  7.90  7.22  6.89  6.89  6.89 10.59
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905.9 906.1 906.3 906.5 906.7 906.9
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INPUT DATA FOR STRONGLY-IMPLICIT PROCEDURE PACKAGE

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      50          5
      1.      .0001           1
```

Hydro-Search, Inc.   HYDROLOGISTS-GEOLOGISTS-ENGINEERS

INPUT DATA FOR OUTPUT CONTROL PACKAGE

```
      -4            -3            77            78
       0             1             1             1
       1             1             1             1
```

APPENDIX B.2

TRANSPORT MODEL INPUT

EXAMPLE INPUT DATA FOR BASIC TRANSPORT PACKAGE

```
REFUSE HIDEAWAY LANDFILL CONTAMINANT TRANSPORT MODEL
  9/27/91        20 ROWS  50 COL.  1 LAYER
              1           20          50              1
SEC FT  RAM
T T T T
 1
           1              1.   (11F6.1)
1702.01135.0 757.0 505.0 337.0 225.0 150.0 100.0 100.0 100.0 100.0
 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0
 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0
 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 150.0
 225.0 337.0 505.0 757.01135.01702.0
           1              1.   (11F6.1)
 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0
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Hydro-Search, Inc.   HYDROLOGISTS·GEOLOGISTS·ENGINEERS

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Hydro-Search, Inc.   HYDROLOGISTS·GEOLOGISTS·ENGINEERS

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Hydro-Search, Inc.   HYDROLOGISTS·GEOLOGISTS·ENGINEERS

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EXAMPLE INPUT DATA FOR ADVECTION PACKAGE

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EXAMPLE INPUT DATA FOR DISPERSION PACKAGE

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        3          1.    (14F5.0)                          -1
10.  10.  30.  10.  10.  10.  10.  10.  10.  10.  10.  10.  10.  10.
10.  10.  10.  10.  10.  10.  10.  10.  10.  10.  10.  10.  10.  10.
10.  10.  10.  30.  30.  30.  30.  30.  30.  30.  30.  30.  30.  30.
30.  30.  30.  30.  30.  10.  10.  10.
10.  10.  30.  10.  10.  10.  10.  10.  10.  10.  10.  10.  10.  10.
10.  10.  10.  10.  10.  10.  10.  10.  10.  10.  10.  10.  10.  10.
10.  10.  10.  30.  30.  30.  30.  30.  30.  30.  30.  30.  30.  30.
30.  30.  30.  30.  30.  10.  10.  10.
10.  10.  30.  10.  10.  10.  10.  10.  10.  10.  10.  10.  10.  30.
30.  10.  10.  10.  10.  10.  10.  10.  10.  10.  10.  10.  10.  10.
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10.  10.  10.  10.  10.  10.  10.  10.  10.  30.  30.  30.  30.  30.
30.  30.  30.  10.  10.  10.  10.  10.
         0           .3
         0           .3
         0          0.
```

EXAMPLE INPUT DATA FOR SINK & SOURCE MIXING PACKAGE

```
F F F F F F
        100
        20
        1           1           16          12.             1
        1           1           17          12.             1
        1           1           18          12.             1
        1           1           19          12.             1
        1           1           20          12.             1
        1           1           21          12.             1
        1           1           22          12.             1
        1           1           23          12.             1
        1           1           24          12.             1
        1           1           25          12.             1
        1           1           26          12.             1
        1           1           27          12.             1
        1           1           28          12.             1
        1           1           29          12.             1
        1           1           30          12.             1
        1           1           31          12.             1
        1           1           32          12.             1
        1           1           33          12.             1
        1           1           34          12.             1
        1           1           35          12.             1
```

EXAMPLE INPUT DATA FOR CHEMICAL REACTION PACKAGE

```
         0           1
03.4881e-08
03.4881e-08
```

APPENDIX C

MODEL MASS BALANCES

APPENDIX C.1

FLOW MODEL

```
VOLUMETRIC BUDGET FOR MODEL AT END OF TIME STEP 1 - STRESS PERIOD 1
-------------------------------------------------------------------

                CUMULATIVE VOLUMES        L**3
                ------------------

                IN:
                ---
                    STORAGE =    0.00000E+00
             CONSTANT HEAD =    0.13563E+08

                 TOTAL IN =     0.13563E+08

                OUT:
                ----
                    STORAGE =    0.00000E+00
             CONSTANT HEAD =    0.13563E+08

                TOTAL OUT =     0.13563E+08

                 IN - OUT =     -105.00

         PERCENT DISCREPANCY =                   0.00
```

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APPENDIX C.2

TRANSPORT MODEL

Hydro-Search, Inc.

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FIGURE 4-1   CUMULATIVE MASS BUDGET

at end of transport step 12, time step 1, stress period
----

	in	out
constant concentration:	0.1695640E+09	-418265.1
constant head:	0.0000000E+00	-0.2959358E-0
decay or biodegradation:	192833.2	-0.1698742E+0
mass storage (solute):	0.6963505E+08	-0.9764038E+0
[total]:	0.2393919E+09	-0.2679329E+09

net (in - out): -0.2854102E+08
discrepancy (percent): -11.25158

FIGURE 4-2   CUMULATIVE MASS BUDGET

at end of transport step 12, time step 1, stress period
----

	in	out
constant concentration:	0.1504114E+10	-3147234.
constant head:	0.0000000E+00	-2494182.
decay or biodegradation:	73041.39	-0.1207096E+10
mass storage (solute):	0.4676766E+09	-0.7211034E+09
[total]:	0.1971864E+10	-0.1933840E+10
net (in - out):	0.3802317E+08	
discrepancy (percent):	1.947058	

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