#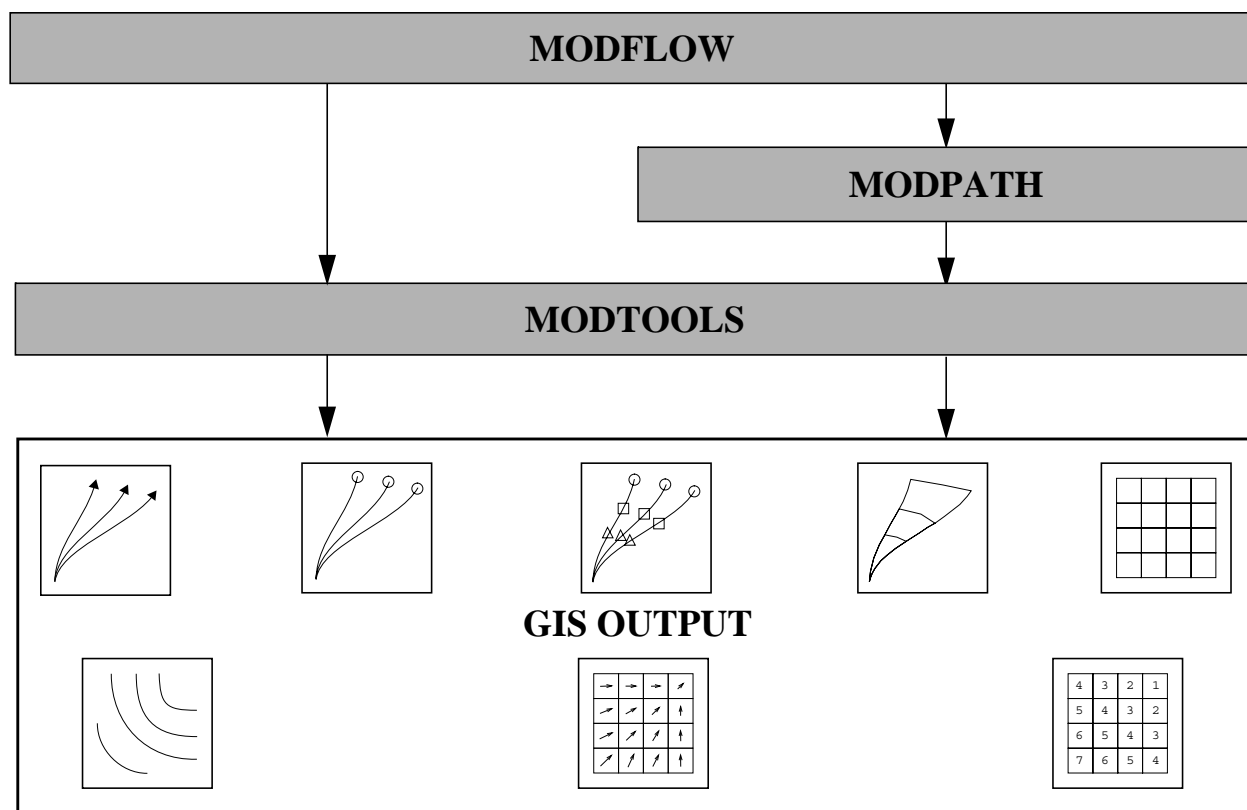 USER'S GUIDE FOR MODTOOLS: COMPUTER PROGRAMS FOR TRANSLATING DATA OF MODFLOW AND MODPATH INTO GEOGRAPHIC INFORMATION SYSTEM FILES

USER'S GUIDE FOR MODTOOLS: COMPUTER PROGRAMS FOR TRANSLATING DATA OF MODFLOW AND MODPATH INTO GEOGRAPHIC INFORMATION SYSTEM FILES

By Leonard L. Orzol

U.S. DEPARTMENT OF THE INTERIOR
BRUCE BABBITT, Secretary

U.S. GEOLOGICAL SURVEY
Gordon P. Eaton, Director

PREFACE

This report presents a version of the computer programs called MODTOOLS for translating data from the U.S. Geological Survey (USGS) modular finite-difference ground-water flow model (commonly known as MODFLOW) and particle-tracking programs (commonly known as MODPATH) into geographic information system (GIS) files. The programs have been tested by using them for a variety of model simulations, but it is possible that other applications could reveal errors. Users are requested to notify the USGS if errors are found in this report or the programs.

Although these programs have been used by the USGS, no warranty, expressed or implied, is made by the USGS or the United States Government as to the accuracy and functioning of the programs and related program material. Nor shall the fact of distribution constitute any such warranty, and no responsibility is assumed by the USGS in connection therewith.

The computer programs are available through the World Wide Web at the address:
http://water.usgs.gov/software/
or by anonymous ftp file transfer from directory /pub/software/ground_water/modtools at the Internet address
water.usgs.gov

The computer programs are also available on diskette for the cost of processing from:

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437 National Center
Reston, VA 20192
Telephone: (703) 648-5695

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USER'S GUIDE FOR MODTOOLS: COMPUTER PROGRAMS FOR TRANSLATING DATA OF MODFLOW AND MODPATH INTO GEOGRAPHIC INFORMATION SYSTEM FILES

By Leonard L. Orzol

Abstract

MODTOOLS is a set of computer programs for translating data of the ground-water model, MODFLOW, and the particle-tracker, MODPATH, into a Geographic Information System (GIS). MODTOOLS translates data into a GIS software called ARC/INFO. MODFLOW is the recognized name for the U.S. Geological Survey Modular Three-Dimensional Finite-Difference Ground-Water Model. MODTOOLS uses the data arrays input to or output by MODFLOW during a ground-water flow simulation to construct several types of GIS output files. MODTOOLS can also be used to translate data from MODPATH into GIS files. MODPATH and its companion program, MODPATH-PLOT, are collectively called the U.S. Geological Survey Three-Dimensional Particle Tracking Post-Processing Programs. MODPATH is used to calculate ground-water flow paths using the results of MODFLOW and MODPATH-PLOT can be used to display the flow paths in various ways.

MODTOOLS uses the particle data calculated by MODPATH to construct several types of GIS output. MODTOOLS uses particle information recorded by MODPATH such as the row, column, or layer of the model grid, to generate a set of characteristics associated with each particle. The user can choose from the set of characteristics associated with each particle and use the capabilities of the GIS to selectively trace the movement of water discharging from specific cells in the model grid. MODTOOLS allows the hydrogeologist to utilize the capabilities of the GIS to graphically combine the results of the particle-tracking analysis, which facilitates the analysis and understanding of complex ground-water flow systems.

INTRODUCTION

MODTOOLS is a set of computer programs for translating data from the popular ground-water modeling programs, MODFLOW and MODPATH, into Geographic Information System (GIS) data files. MODTOOLS translates data into a GIS software called ARC/INFO. MODFLOW can simulate ground-water flow in a three-dimensional heterogeneous and anisotropic medium (McDonald and Harbaugh,

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1988). MODPATH is a particle tracking post-processing program designed to work with MODFLOW. MODPATH can compute the movement of hypothetical water particles through the simulated ground-water flow system (Pollock, 1994). Geographic Information Systems are effective tools for storing, managing, and displaying the types of spatial data often used in ground-water modeling analyses. The graphical, statistical, and database capabilities of the GIS provide powerful tools for the analysis of model data and results. Geographic Information Systems are useful tools to construct input data or to display output data from ground-water model simulations. An example of a ground-water modeling study that used a GIS is that of Morgan and McFarland (1994). MODTOOLS was used to help analyze the results of this same study to evaluate ground-water vulnerability (Snyder and others, 1996) and for comparison with chlorofluorocarbon age dating (Hinkle and Snyder, in press).

The use of a GIS enables the graphical combination of output from MODFLOW and MODPATH with other spatial data, which facilitates the analysis and understanding of complex ground-water flow systems and evaluation of the impact of human activities. MODPATH-PLOT (Pollock, 1994), the graphical companion program of MODPATH, has a variety of options for displaying results from MODPATH and MODFLOW, but does not have the power of a full-featured GIS for spatial analysis. Also, MODTOOLS has features that enables it to produce GIS data files compatible with those produced by MODFLOWARC, a modified version of MODFLOW that reads and writes to GIS files (Orzol and McGrath, 1992).

This report documents MODTOOLS and serves as a user's manual for operating MODTOOLS. Possible uses of MODTOOLS are demonstrated in eight examples. All instructions necessary to reproduce these examples are listed in Appendix B. The report also includes a "quick-start guide" listing the basic instructions for operating MODTOOLS, a detailed discussion of the program menus, descriptions of GIS files output by MODTOOLS, and instructions for installing MODTOOLS.

Acknowledgments

I would like to thank report team members Dave Morgan, Daryll Pope, John Williams, and Bill McFarland of the U.S. Geological Survey (USGS) for their helpful comments and especially acknowledge Dan Snyder (USGS) for his contribution to this project. I would also like to thank Arlen Harbaugh and Dave Pollock of the USGS Office of Ground Water for their suggestions.

CREATING GEOGRAPHIC INFORMATION SYSTEM OUTPUT USING MODTOOLS

MODTOOLS creates eight major types of GIS output from data of MODPATH and MODFLOW. The types of GIS output are listed in table 1 and their relations to MODFLOW, MODPATH, and MODTOOLS are shown in figure 1. The GIS output consists of particle and model-grid coverages (the spatial arrangement of points, lines, or polygons) and INFO files, which contain characteristics associated with the appropriate particle or cell. There are four types of GIS output created from the particle data output by MODPATH: pathline, endpoint, time-series, and zones of transport. A fifth type

of GIS output is created from the input data to MODPATH defining the physical dimensions of the model grid and is called model-grid GIS output. Three types of GIS output are created from data of MODFLOW: contour, velocity vector, and cell values. In addition, MODTOOLS can utilize any data in array format to create GIS output.

Table 1. Types of GIS output possible with MODTOOLS

Source	Types of GIS output	Description
MODPATH	PARTICLE PATHLINES	Pathline GIS output is constructed from particle data describing particle paths recorded by MODPATH in the PATHLINE file. This output consists of a set of lines which represent each particle path.
	PARTICLE ENDPOINTS	Endpoint GIS output is constructed from particle data describing the starting or final positions of particles recorded by MODPATH in the ENDPOINT file. This output consists of points which represent the starting or final positions of each particle.
	PARTICLE TIME-SERIES	Time-series GIS output is constructed from particle data describing particle locations at specified model time steps recorded by MODPATH in the TIMESERS file. This output consists of points that represent the positions of each particle along the particle path at specified times of travel.
	ZONES OF TRANSPORT	Zones-of-transport (ZOT) GIS output is constructed from particle data describing particle locations at specified model time steps recorded by MODPATH in the TIMESERS and ENDPOINT files. This output consists of polygons representing the projection of the zones of transport onto the user-specified plane of the model grid.
	MODEL GRID	Model-grid GIS output is constructed from data arrays defining the model-cell geometry input to MODPATH. This output consists of polygons that represent the cell faces of the user-specified plane of the model grid.
MODFLOW	CONTOURS OF INPUT AND OUTPUT ARRAYS	Contour GIS output is constructed from data arrays of MODFLOW or arrays gridded to same scale as the MODFLOW grid. This output consists of lines connecting points of equal value.
	VELOCITY VECTORS	Velocity-vector GIS output is constructed from the head values and cell-by-cell flow terms output by the Basic and Block Centered Flow Packages of MODFLOW. Velocity-vector output consists of lines indicating the direction and magnitude of simulated ground-water velocity.
	CELL VALUES	Cell-value GIS output is constructed from data arrays of MODFLOW or arrays gridded to same scale as the MODFLOW grid. This GIS output consists of records in GIS files that contain the values of the specified data arrays corresponding to model-grid cells.

MODTOOLS incorporates all the types of output options of MODPATH-PLOT, but has several capabilities not found in MODPATH-PLOT. Both MODTOOLS and MODPATH-PLOT can create output in both mapview and vertical profile orientations. MODPATH-PLOT vertical profiles, however, can be viewed only along rows or columns, whereas MODTOOLS can construct GIS output of a profile view along a specified particle pathline. Another capability of MODTOOLS that is not available in MODPATH-PLOT is creation of zones of transport GIS output from particle data output by MODPATH. Zones of transport are the volumes of an aquifer that recharge or contribute water to a well or well field for specific times of travel (U.S. Environmental Protection Agency, 1987).

MODTOOLS can produce mapview GIS output of contour lines like MODPATH-PLOT, but the user has the additional option of viewing the contours in a vertical profile orientation along a row or column of the model grid. Another type of GIS output created by MODTOOLS is velocity vectors that show the direction and magnitude of ground-water velocity within each model cell. MODTOOLS can

MODFLOW

GROUND-WATER

FLOW MODEL

MODPATH

PARTICLE

TRACKING MODEL

MODTOOLS

Particle Pathlines

Particle Endpoints

Particle Time-series

Zones of transport

Model grid

Contours of input and output arrays

Velocity vectors

Cell values
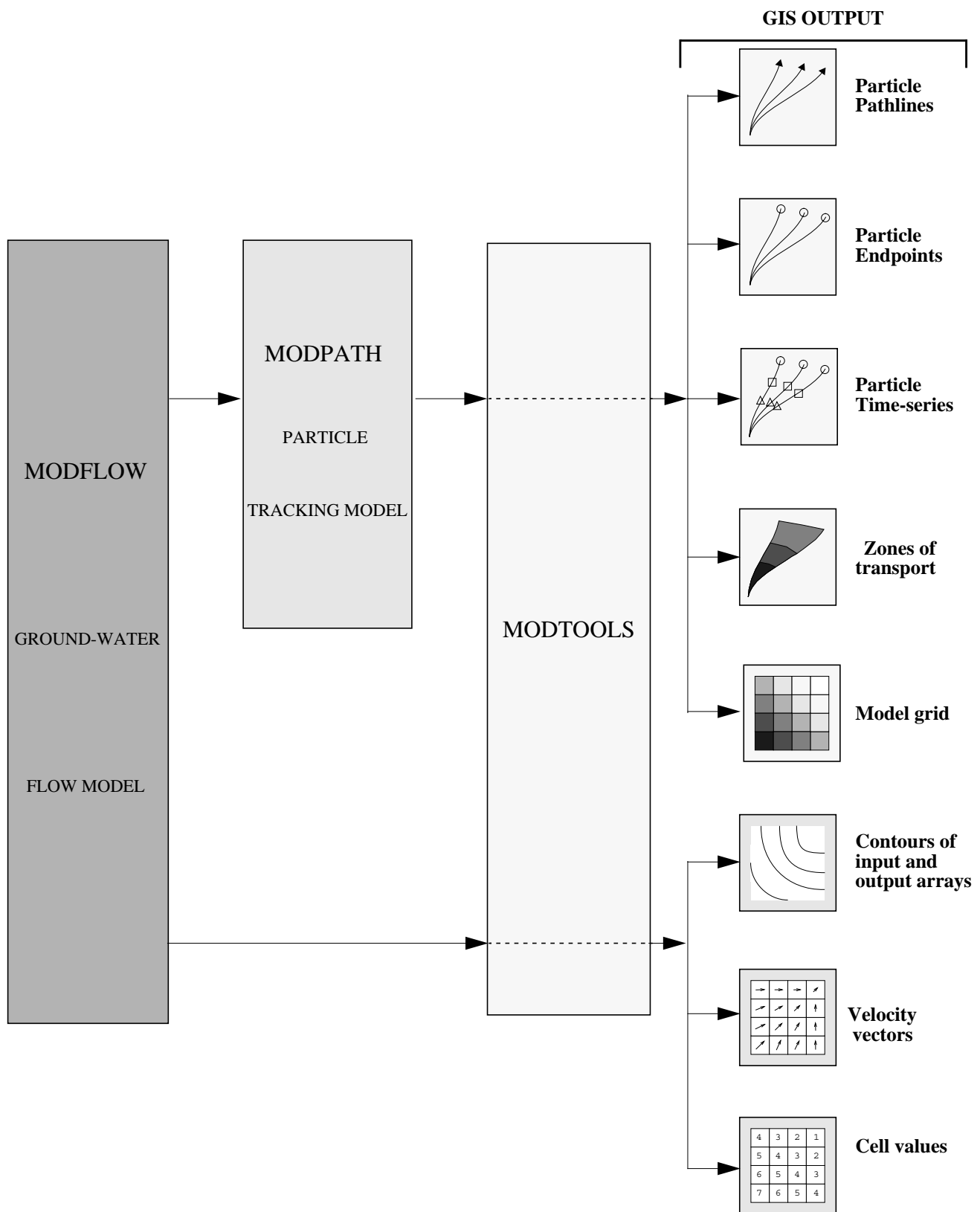
Figure 1. The functional relation between MODFLOW, MODPATH, and MODTOOLS, and GIS output that can be produced by MODTOOLS.

also create GIS output from the output data arrays of MODFLOW corresponding to model-grid cells, such as the head and drawdown values output by the Basic Package or cell-by-cell flow terms from other stress packages in MODFLOW. Examples of the eight types of GIS output available from MODTOOLS are illustrated in the following sections. The examples were developed using the sample problem in Pollock (1994).

Description of Sample Problem Used in Examples

The hypothetical flow system used as a sample problem in these examples is from Pollock (1994) and is illustrated in figure 2. The flow system consists of two aquifers separated by a 20-foot-thick confining layer. Recharge to the system is uniformly distributed over the water table at a rate of 0.0045 feet per day. Discharge is to a partially penetrating river along the right side of the flow system in the upper aquifer and to wells.

Two simulations were used in the examples. In the first simulation (problem 1 of Pollock [1994, p 6–4]), steady-state conditions were simulated with one pumping well, which is located in the lower aquifer and discharges at 80,000 cubic feet per day. In the second simulation (problem 2 of Pollock [1994, p. 6–15]), transient conditions were simulated after the addition of a second well discharging from the upper aquifer immediately above the well in the lower aquifer (fig. 2). The transient MODFLOW simulation was divided into three stress periods. Stress period 1 was 500 years long with one time step. During stress period 1, only one well was present in layer 4 and all stresses were identical to those of the steady-state simulation. Stress period 2 was 30 years long and consisted of eight time steps. During stress period 2, wells present in layers 1 and 4 each discharged at 80,000 cubic feet per day. Stress period 3 was 1,250 years long and consisted of one time step. Both wells continued to discharge at 80,000 cubic feet per day during stress period 3.

The system was simulated using a finite-difference grid containing 27 rows, 27 columns, and 5 layers. Horizontal grid spacing varied from 40 foot by 40 foot squares at the wells to 400 foot by 400 foot squares away from the wells. The upper unconfined aquifer was simulated by one layer. The confining unit was represented implicitly using a quasi-three-dimensional layer and a vertical leakance coefficient. The lower aquifer was represented by four 50-foot-thick layers. Both wells were located in row 14, column 14. The well in the lower aquifer was located in model layer 4.

Output Options for MODPATH Data

MODPATH computes particle locations for particle pathlines, starting or final positions, and time-series positions at selected times of travel. MODTOOLS uses these particle locations to create GIS output. In addition to particle locations, MODPATH records characteristics such as the row, column, and layer of each model cell the particle has entered. MODTOOLS associates these characteristics with the appropriate particle in the GIS output. These characteristics can be used to identify specific particles in the analysis of particle-tracking results.
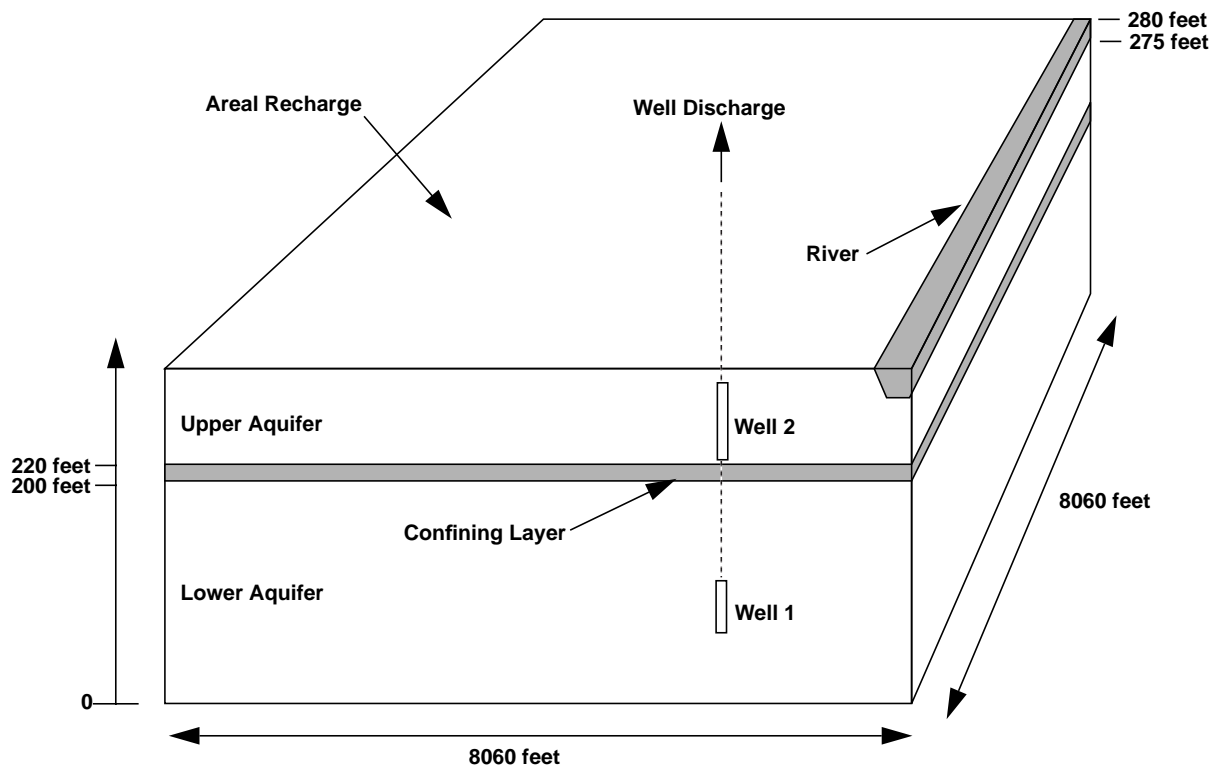
Figure 2. Diagram of hypothetical flow system simulated in examples (modified from Pollock, 1994, p. 6–2).

The files necessary to reproduce examples 1 through 5 are listed in Appendix B; a listing of the menu responses necessary to create the GIS output for these five examples is also included.

Example 1: Particle Pathlines

MODPATH provides the option to record the locations of particles along pathlines. This option is called a pathline analysis (Pollock, 1994). A pathline analysis is useful to illustrate the movement of water within a flow system. MODTOOLS uses the particle data recorded by MODPATH in the PATHLINE file (Pollock, 1994) to construct GIS output consisting of lines that represent the particle pathlines. Example 1 (fig. 3) combines the GIS output from the results of four particle-tracking analyses. This example was taken from the transient simulation and shows a pathline analysis for well 2 in mapview using the backward-tracking mode of MODPATH (see Pollock, 1994, problem 2, run 1, p. 6–5 to 6–18). Well 2 begins pumping at a simulation time of 500 years. A pair of particles was started from the cell that contains well 2 (row 14, column 14, layer 1) at four points in time and the particles were tracked backward in the reverse direction of ground-water flow. The user must run MODPATH four times to produce particle data at the four simulation times, 500, 501, 503, and 510 years. After each particle-tracking analysis using MODPATH, the user would then create pathline GIS output using MODTOOLS.

Using the capabilities of the GIS, the user is able to overlay the GIS output from MODTOOLS of the four pathline analyses and to distinguish the pathlines from each analysis with a different line symbol (fig. 3). For illustrative purposes arrows to indicate the direction of ground-water flow were added to
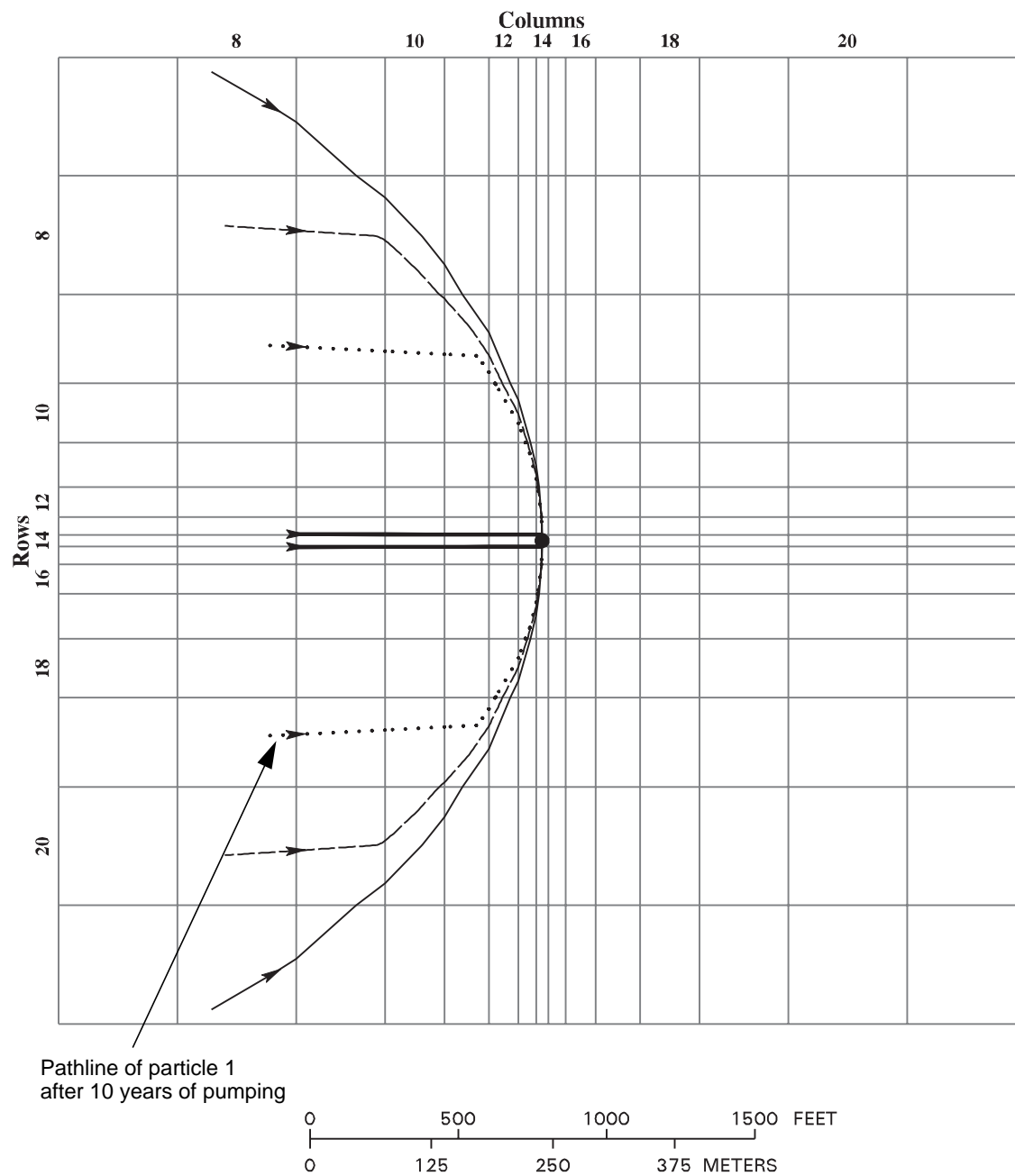
Figure 3. Simulated pathlines resulting from backward tracking of two particles from well 2 under transient conditions (see Appendix B, example 1).

each particle pathline, and a dot was added to show the location of well 2. These lines represent the paths taken by water discharging to well 2 at the start of pumping in layer 1, after 1 year of pumping, after 3 years of pumping, and after 10 years of pumping. The shape and direction of the pathlines indicates the progressive changes of the ground-water system through time caused by pumping of well 2. The sharp bends in the pathlines correspond to the time at which pumping began in layer 1.

Example 2: Particle Endpoints

MODPATH provides the option to record the starting or final locations of particles from a particle-tracking analysis. This option is called an endpoint analysis (Pollock, 1994). An endpoint analysis is useful in delineating sources of water to major discharge points such as rivers and wells or to any location within a flow system. MODTOOLS uses particle data recorded by MODPATH in the ENDPOINT file (Pollock, 1994) to produce a GIS output consisting of points which represent starting or final locations of particles and up to 30 characteristics associated with each particle.

Example 2 (fig. 4) uses the transient simulation and shows an endpoint analysis for wells 1 and 2 in mapview using the forward-tracking mode of MODPATH (see Pollock, 1994, problem 2, run 3, p. 6–20 to 6–21). The system has attained a new hydraulic steady state by the end of stress period two. Four particles were placed at the water table in each cell in layer 1 at the beginning of stress period 3 (simulation time equals 530 years), and the particles were tracked forward in the direction of the ground-water flow. The GIS output produced by MODTOOLS consists of 2,808 points, which represent the starting locations of the particles that discharged to either of the two wells.

In this endpoint analysis (fig. 4), characteristics associated with each particle were used to identify only those particles discharging to wells 1 and 2. Creation of the endpoint plot for this example using MODPATH-PLOT (Pollock, 1994, page 6–21) required the creation of a zone code array (Pollock, 1994) in order to distinguish and shade locations of the starting points for the particles discharging to the two wells, which is unnecessary for MODTOOLS.

Example 3: Particle Time Series

MODPATH provides the option to record the locations of particles at specific points in time. This option is called a time-series analysis (Pollock, 1994). A time-series analysis is useful to track the migration of particles at specific points in time. MODPATH also has the capability to release a stream of particles over a specified period of time. Combining a multiple particle release with time-series analysis allows the user to track a plume of particles which is helpful for both steady-state and transient simulations. MODTOOLS uses particle data recorded by MODPATH in the TIMESERS file (Pollock, 1994) to produce GIS output consisting of points that represent the locations of particles at specified times of travel; each point has 62 characteristics, such as present time, cumulative travel time, and velocity.

Figure 4. Capture areas for pumping wells 1 and 2 (see Appendix B, example 2).

Example 3 (fig. 5) uses the steady-state simulation and shows a time-series analysis with multiple particle release using the forward-tracking mode of MODPATH (see Pollock, 1994, problem 1, run 4, p. 6–13 to 6–14). Particles were released every 0.5 years for 10 years at the water table in columns 8 and 9 of row 14. Viewed in profile along row 14, the movement of the particle plume towards the well and the river over time can be easily visualized. The locations of particles at specified times of travel are identified by using the GIS to select particles having corresponding cumulative times of travel. In this example, particles were selected for times of travel of 10, 20, 25, and 35 years. These plots give a visual representation of the plume as it moves vertically and laterally through the system. Note how the plume eventually splits into two parts, with one part discharging toward the well and the other to the stream.

Example 4: Zones of Transport

MODTOOLS provides an option for projecting the delineations of zones of transport for discharge features such as wells, streams, or springs onto a two-dimensional surface, such as the water-table layer. (A zone of transport is a volume within a ground-water system that contributes water to a discharge feature for a specific time of travel.) This option is called a zone of transport analysis. The delineation of zones of transport is one of several methods used to assist with delineating wellhead protection areas for wells (U.S. Environmental Protection Agency, 1987). The approach used in MODTOOLS to delineate the zones of transport is documented in Appendix C. MODTOOLS constructs two GIS outputs for this option using particle data recorded by MODPATH in the TIMESERS and ENDPOINT files (Pollock, 1994). The first GIS output is the polygons that result from projecting the zones of transport for specified times of travel onto a two-dimensional surface (user specified plane), such as the water table. The resulting polygons are not necessarily equivalent to recharge or source areas, because the particle positions used to delineate the zones of transport may be several tens or hundreds of feet beneath the water table. The second GIS output is the points that form the vertices of the polygons. This GIS output contains information about the particles used to delineate the zones, such as elevation or position within the model grid. A zone of transport analysis can be done for a particle-tracking analysis only by using the time-series option for particle output and the backward-tracking mode of MODPATH.

Example 4 (fig. 6), a zone of transport analysis, used the steady-state simulation (see Pollock, 1994, problem 1, run 2, p. 6–10); however, particles were tracked using the time-series option instead of the endpoint option used by Pollock (1994). Particles were arranged as described in Appendix C for the cell containing well 1 (row 14, column 14, layer 4) and were tracked backward toward the cells where the water recharged the ground-water system. Particle data output by MODPATH was recorded every 5 years for times of travel up to 50 years (10 model time steps). The mapview of the 10, 20, 25, and 35 year zones of transport is shown in figure 6. The approach used by MODTOOLS to delineate the zones of transport approximates these zones from particle positions. This approach can sometimes produce noticeable inflections in the boundaries of the zones of transport that are caused by limitations of the
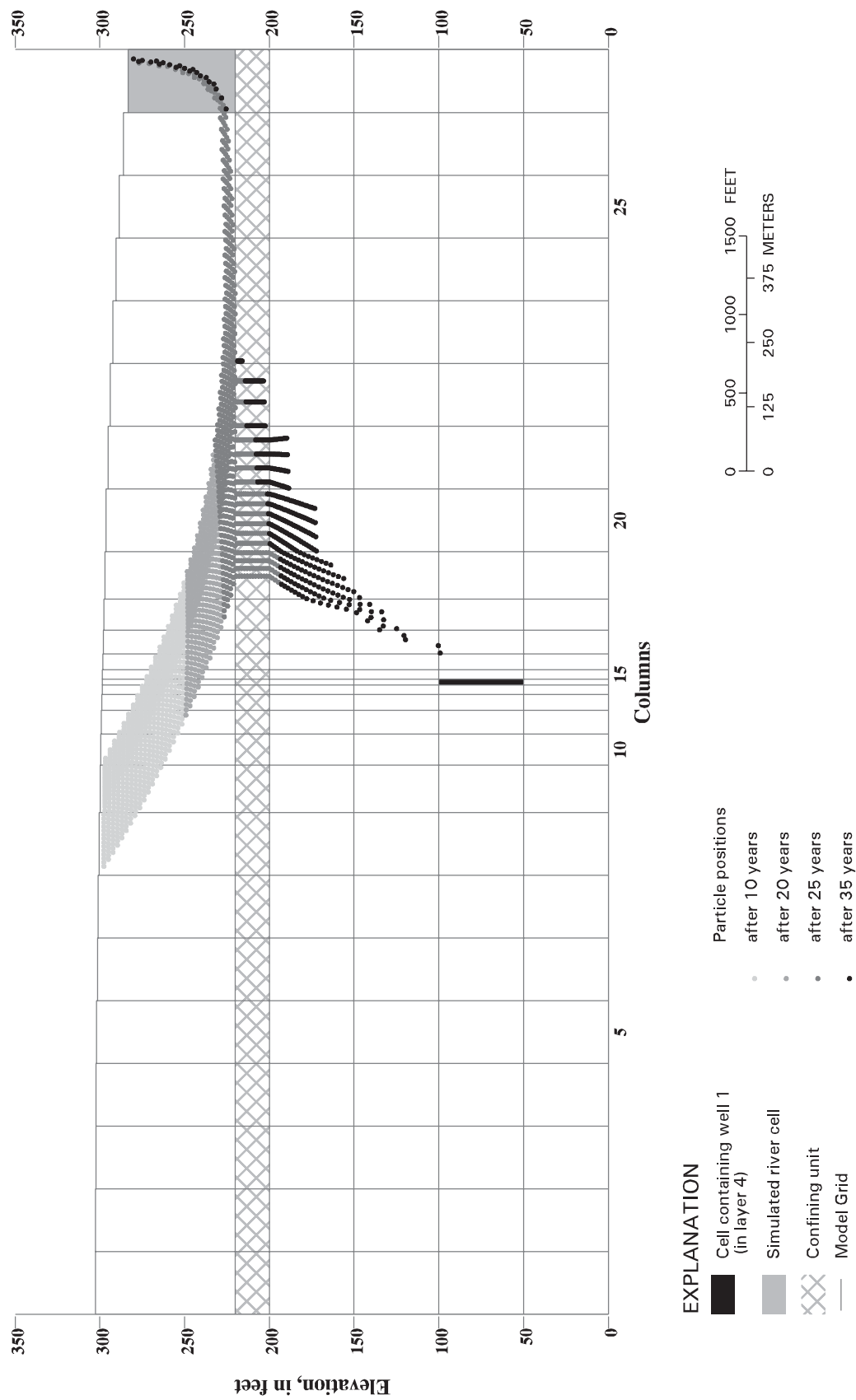
Figure 5. Vertical profile view along row 14 showing the movement of a particle plume formed by a simulated 10 years of continuous release of particles at the water table under steady-state flow conditions (see Appendix B, example 3).

EXPLANATION

Cell containing well 1 (in layer 4)

Simulated river cell

Confining unit

Model Grid

Particle positions

after 10 years

after 20 years

after 25 years

after 35 years

Elevation, in feet

Columns

method used to delineate zones of transport (see Appendix C). In figure 6, the triangular inflections in the boundaries of the zones of transport delineated in the downgradient direction are due to one or more of these limitations.

Example 5: Model Grid

MODTOOLS provides an option to construct GIS output of the model grid in mapview or in vertical profile view along a specified row, column, or particle pathline. This option is most useful for creating a model grid for use in displaying other GIS output in mapview or profile view on row, column, or pathline plots. MODTOOLS uses the data arrays defining grid dimensions from the MAIN file for MODPATH (Pollock, 1994). To create GIS output of a vertical profile view along a particle pathline, the user must first make a particle pathline analysis for which MODTOOLS constructs a pathline GIS output for the specified particle. For a mapview or a vertical profile view along a model row or column, the user need only construct the MODPATH MAIN file. For vertical profile views, MODTOOLS uses the values of the simulated head for the tops of the cells in layer 1 if layer 1 is a water-table layer.

Example 5 (fig. 7) illustrates the use of MODTOOLS to create vertical profile model-grid GIS output. A pathline analysis for well 2 in stress period 2 of the transient simulation was made using the backward-tracking mode of MODPATH (see Pollock, 1994, problem 2, run 1, p. 6–15 to 6–18). MODTOOLS was used to construct a model-grid GIS output in vertical profile view along the pathline of particle 1 and a pathline GIS output of the pathline of particle 1 both of which are shown in figure 7. Particle 1 was started after 10 years of simulated pumping from well 2 in row 14, column 14, layer 1. MODPATH records the particle positions when the particle enters a new cell and at intermediate points whenever the cumulative time of travel corresponds to (1) a user-specified point in time, or (2) the end of a MODFLOW time step in a transient simulation (Pollock, 1994). MODTOOLS used the head values from the beginning of stress period 2 as the tops of the cells in layer 1.

Output Options for MODFLOW Data

MODTOOLS provides three options to construct GIS output from the data arrays of MODFLOW. These options are useful for displaying MODFLOW input and output data with other spatial data in the user's GIS, such as streams or geology. The first option allows the user to construct GIS output of contour lines using data arrays, such as head, drawdown, or cell-by-cell flow terms. The second option allows the user to construct velocity vectors representing the magnitude and direction of ground-water velocity in each active cell of the model grid. The third option allows the user to construct GIS files from the data arrays of MODFLOW; data in the files can be displayed or plotted with other GIS data, such as the model grid.

The files necessary to reproduce examples 6 through 8 are listed in Appendix B; a listing of the menu responses necessary to create the GIS output for these three examples is also included.
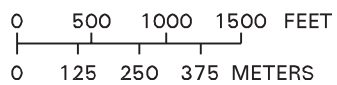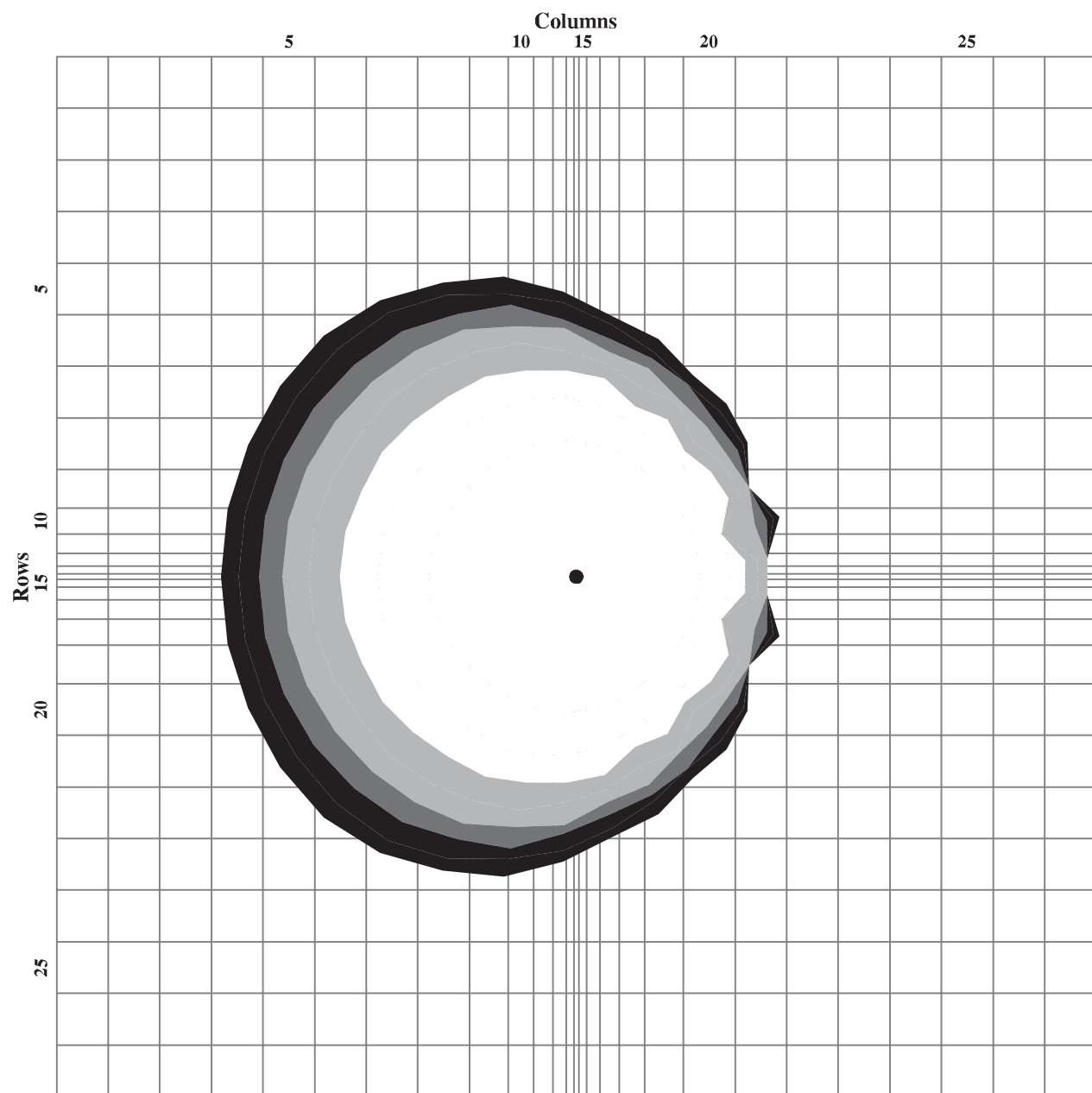
Figure 6. Zones of transport for 10, 20, 25, and 35 years for well 1 (see Appendix B, example 4).

Elevation, in feet

350
300
250
200
150
100
50
0

| 14 | 14 | 14 | 13 | 13 | 12 | 12 | 11 | 10 | 9 | 8 |
| 15 | 16 | 17 | 17 | 18 | 18 | 19 | 19 | 19 | 19 | 19 |

Columns
Rows

0   50   100   150   METERS
0   200   400   600   FEET

EXPLANATION

Cell containing well 2

—— Particle pathline

—— Model grid along pathline

➤ Direction of ground-water flow

Figure 7. A vertical profile view of the model grid and pathline traveled by particle 1 (see Appendix B, example 5) (see figure 3 for pathline of particle 1 in mapview).

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Example 6: Contour lines of values in Input and Output Arrays

MODTOOLS provides an option to construct GIS output consisting of lines connecting points of equal value (contour lines) from the cell-by-cell terms of MODFLOW. This option is useful in producing contours of MODFLOW data, such as the simulated head values, in a GIS format that can be displayed or plotted with other GIS data. One option would be to graphically overlay lines of equal observed head with the lines of equal simulated head to facilitate model calibration.

Figure 8 illustrates contour GIS output showing lines of the equal simulated head for cells in layer 4. Two types of GIS output were used to create this figure: (1) lines of equal hydraulic head constructed by MODTOOLS using the simulated steady-state head values output by MODFLOW, and (2) model grid in mapview.

Example 7: Velocity Vectors

MODTOOLS provides an option to construct GIS output consisting of velocity vectors showing the magnitude and direction of simulated ground-water movement in the active cells of the model grid. This option is useful in displaying the results of a ground-water flow simulation, for checking hypotheses regarding the magnitude and direction of water movement, and for identifying potential ground-water flow paths. To produce this type of GIS output, the user must make a MODFLOW simulation and assemble the MODPATH MAIN file (MODPATH does not need to be run). Data required to construct a velocity-vector GIS output include grid dimensions and porosity arrays used by MODPATH, and the simulated head and cell-by-cell flow terms output by the Basic and the Block Centered Flow Packages of MODFLOW.

Figure 9 illustrates velocity-vector GIS output. The velocity vectors, representing the magnitude and direction of ground-water velocity in layer 4, were generated for the steady-state simulation. The direction of ground-water flow is computed from the x and y components of the cell-by-cell flow terms. The length of the vector indicates the relative magnitude of ground-water velocity, which is based on the rates of flow through the cell faces, the wetted cross-sectional area of the faces, the porosity of the material in the cell, and a user-specified scaling value. This part of MODTOOLS was adapted from the work of Scott (1990).

Example 8: Cell Values

MODTOOLS provides an option to construct GIS output from the data arrays of MODFLOW. This option is useful in translating MODFLOW data into a GIS format that can be displayed or plotted with other GIS data, such as the locations of pumping wells, streams, or cultural features.

For example 8 (fig. 10), the simulated head values and the data defining the cell dimensions in the MODPATH MAIN file were used to construct GIS output for a vertical profile of the heads and model grid along row 14. Values of simulated head in layer 1 for stress period 3 at time step 1 from the transient simulation were used for this example. MODTOOLS used the simulated head values for stress period 1, time step 1 for the tops of the cells in layer 1. The values of simulated head for layer 1 were selected
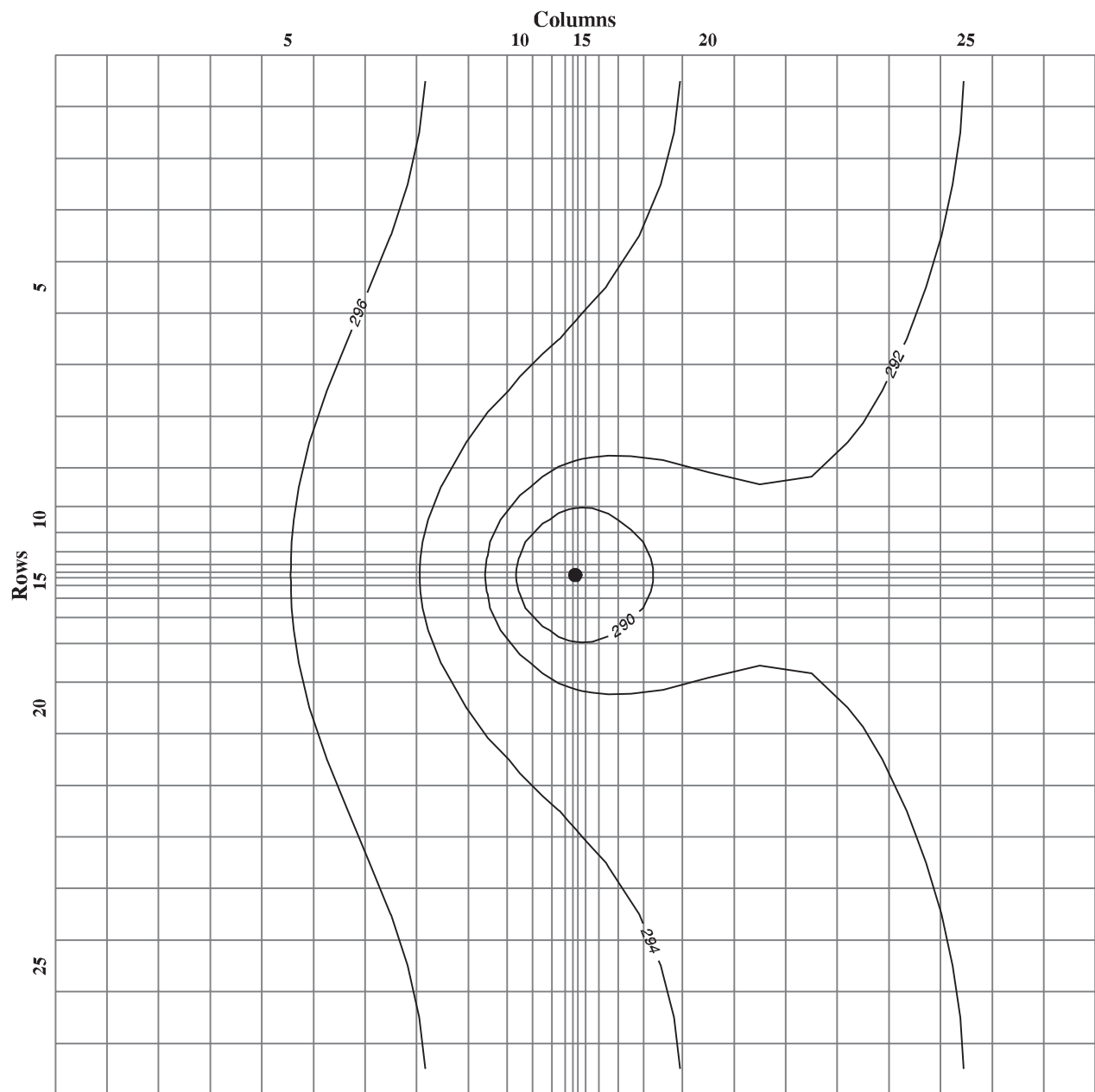
Figure 8. Lines of equal simulated hydraulic head for cells in layer 4 (see Appendix B, example 6).

Columns

Figure 9. Horizontal velocity vectors for layer 4 (see Appendix B, example 7).
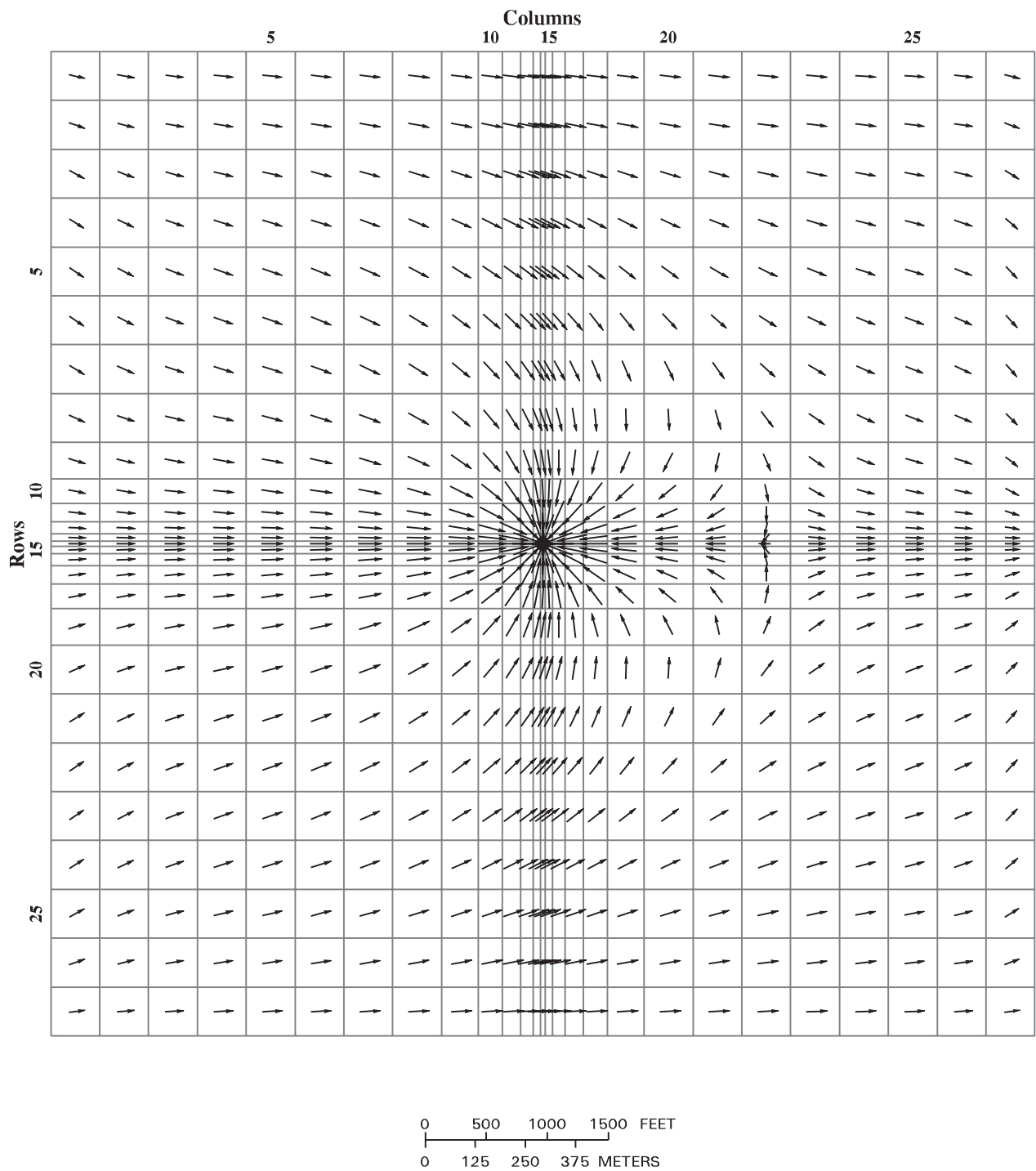
EXPLANATION

⟵⟶ Flow vector (length scaled logarithmically)

⟶ Model grid

● Well 1 (in layer 4)

using the GIS and are shown in figure 10 as a solid line. The differences in elevation between the tops of the cells in layer 1 and the solid line drawn in each cell are the simulated drawdown between the end of stress period 1, time step 1 and the end of stress period 3, time step 1.

MODTOOLS USER'S GUIDE

Overview of MODTOOLS

The set of MODTOOLS computer programs consists of a main AML (Arc Macro Language) program called MODTOOLS.AML, a main FORTRAN program called MODTOOLS.F, a large number of FORTRAN subroutines, and two secondary AML programs. The primary purpose of the MODTOOLS.AML program is to manage the process of constructing GIS output from the particle and array data of MODPATH and MODFLOW. Subsequently, MODTOOLS.AML passes control to MODTOOLS.F and other FORTRAN programs. The primary purpose of the FORTRAN programs is the creation of features such as particle pathlines or the model grid in a GIS format. The particle and array data are stored in a single, one-dimensional master array that can be adjusted to accommodate large simulations simply by changing its dimension in the MODTOOLS.F program. The primary purpose of secondary AML programs is the creation of GIS features.

MODTOOLS obtains data from a combination of file and interactive keyboard input. Files containing the basic information describing the flow system, such as geometry, boundary conditions, and the cell-by-cell flow terms, are referred to as "flow system files." Interactive keyboard input is used primarily to supply information about GIS output options that change frequently. Keyboard input is recorded in a special batch file called MODTOOLS.OUT. A batch file generated from a previous MODTOOLS session can be used in place of keyboard input.

The user's guide part of this report is organized into several sections:
(1) a "quick-start guide" that briefly describes the overall process of using MODTOOLS with MODFLOW and MODPATH to produce GIS output,
(2) instructions for constructing the NAME file required by MODTOOLS to open and close files,
(3) instructions for using MODTOOLS in batch mode,
(4) a discussion of coordinate systems used in MODTOOLS,
(5) a description of MODTOOLS error messages and common errors,
(6) a description of the menu and response system for interactive input, and
(7) a description of GIS output file structure and content.

A Quick-Start Guide to Running MODTOOLS

Five basic steps are necessary to generate GIS output using MODTOOLS. To generate GIS output from MODPATH results, all five steps must be followed. If the user is generating only GIS output of MODFLOW *output* (contour lines, velocity vectors, or cell values), then step 3 (running MODPATH)

EXPLANATION

Cells containing well 1 (in layer 4) and well 2 (in layer 1)

Simulated head in layer 1 for stress period 3, time step 1
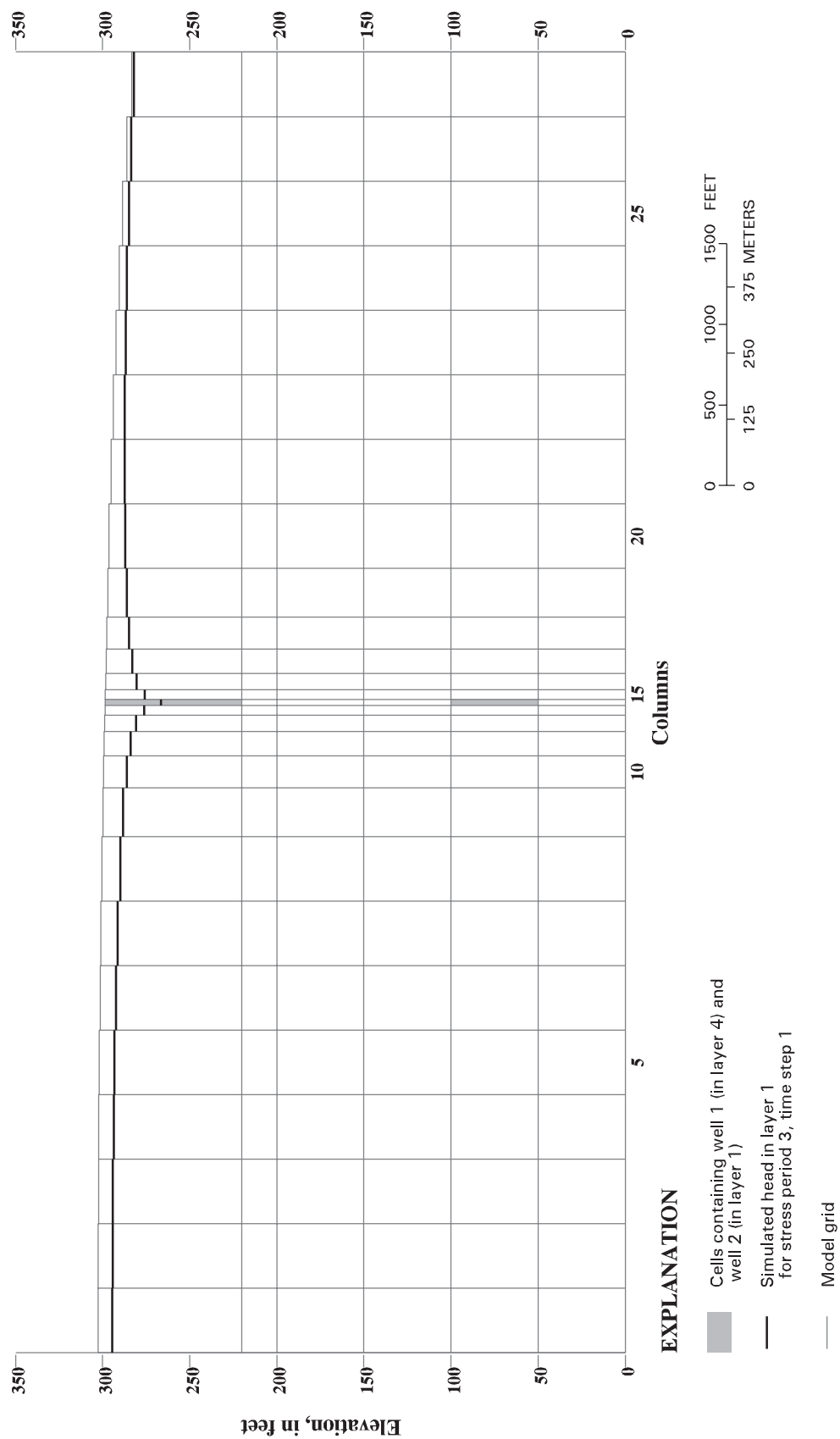
Model grid

Figure 10. Vertical view along row 14 showing model grid and simulated heads (see Appendix B, example 8).

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can be omitted. If the user is generating only GIS output of MODFLOW *input* (contours or cell values), then steps 1 and 3 can be omitted. For more detailed instructions on using MODFLOW and MODPATH, the user may refer to McDonald and Harbaugh (1988) and Pollock (1994), respectively. Instructions for obtaining and installing MODTOOLS are given in Appendix A.

Step 1. Run MODFLOW (see Pollock, 1994, p. 3–4)

MODPATH computes velocity components using the cell-by-cell flow information generated by MODFLOW. Before MODPATH can be run, MODFLOW must be run and cell-by-cell output written to a file. MODPATH also requires MODFLOW head output for any layer that can have a water table within it.

Step 2. Assemble MODPATH Data Files (see Pollock, 1994, p. 3–4)

MODPATH always requires the following data files:

(1) Flow System Files -- MODFLOW and MODPATH data files that contain information about the physical dimensions of the ground-water system, boundary conditions, hydrologic properties, and output heads and cell-by-cell flows.

(2) NAME File -- A data file containing a list of input and output files required by MODPATH, FORTRAN unit numbers, and file-type descriptions. This information is used by MODPATH and MODTOOLS to open the files.

Step 3. Run MODPATH (see Pollock, 1994, p. 3–4)

Once the necessary data files have been prepared, MODPATH can be executed using the methods summarized by Pollock (1994, p. 3–4 to 3–5).

Step 4. Run MODTOOLS

The user must first initiate the ARC/INFO GIS software by issuing the appropriate command at the UNIX prompt. On many computer systems the command is simply,

arc

The user then issues the ARC/INFO system command that specifies the path to the directory where the MODTOOLS.AML program is stored. This command informs the ARC/INFO software to search the directory *[path]* first when a command is issued to execute an ARC/INFO AML program.

&amlpath [path]

 The user is now ready to run the MODTOOLS program by issuing the **&run** command followed by the name of the AML program to run, **modtools**, and a list of arguments expected by the MODTOOLS programs:

&run modtools <GIS output> <NAME file> {batch file}

Two arguments, the name for the GIS output and the name of the **NAME file**, are mandatory. The NAME file contains a list of the files that will be read by MODTOOLS. These files contain data describing particle locations and characteristics associated with each particle, model-cell geometry, and other pertinent information. The third argument, the name of a **batch file** containing a list of menu responses for MODTOOLS to create GIS output, is optional. Use of a batch file eliminates the need to interactively answer the menu responses over and over again for similar runs. Use of the batch file is described in a later section.

MODTOOLS creates a file called MODTOOLS.LIST, which contains a listing of all operations preformed by MODTOOLS. This file is important, because MODTOOLS records any errors to this file. The user should review this file first if MODTOOLS does not properly produce the specified GIS output.

General Instructions

NAME File

The NAME file contains one line for each input data file. This file provides the information needed to manage the input data files. Each line of the NAME file consists of 3 items: (1) a character string signifying the type of data file (table 2), (2) an integer file unit number, and (3) the file name. The NAME file input is read using a free format. Any valid file unit number for a given operating system may be specified. However, MODTOOLS reserves unit numbers in the range of 80 to 99 for internal use. Files can be specified in any order. A typical NAME file for MODTOOLS is shown below:

MAIN   11 main.dat
DATA   31 ibound.1
BUDGET   50 budget.out
HEAD(BINARY) 60 head.out

The first item on each line is a keyword that identifies the type of data file. The character string identifier can be in upper or lower case. MODTOOLS uses the same naming convention as used by MODPATH and MODPATH-PLOT to indicate specific data files (table 2) (Pollock, 1994, p. A–6 to A–7). Ancillary data files usually contain large arrays that are referenced by array control records in other data files. Ancillary data files always must be declared as type DATA. For example, the IBOUND array for each layer of a model might be stored in separate files and only the array control records referenced in the MAIN file. Each file would be assigned a unit number and identified using the keyword DATA in the NAME file.

The naming conventions for the NAME file used by MODTOOLS are summarized in table 2 along with the data file requirements. Because MODTOOLS does not compute particle pathlines, many of the data arrays are not needed by MODTOOLS to create GIS output. MODTOOLS uses two files identified by the keywords CONTOUR-DATA and CONTOUR-CONTROL to create GIS output of contour lines. MODTOOLS allows the user to construct contour lines of miscellaneous gridded model data, such as hydraulic conductivity. The data can be provided in a standard ASCII text file (like the MODPATH-PLOT option of Pollock [1994, p. 4–16]) or in a binary (unformatted) file. MODTOOLS identifies the data using the keyword CONTOUR-DATA. MODTOOLS requires a file identified by the keyword CONTOUR-CONTROL to determine the location and format of the data to be contoured (see "Format of Array Menu" [p. 48] or Pollock, 1994, p. A–2 to A–5). MODTOOLS provides an option for reading head and drawdown values from standard ASCII text files. These values may have been produced by MODFLOW–96 (Harbaugh and McDonald, 1996) or other means, such as by GIS techniques. MODTOOLS requires a file identified by the keyword HEAD-CONTROL to determine the location

Table 2. Summary of data file requirements for MODPATH, MODPATH-PLOT, and MODTOOLS (adapted from Pollock, 1994, p. A–7)

Description	Type of data file Keyword	Needed for MODPATH?	Needed for MODPATH-PLOT?	Include in NAME file?	Needed for MODTOOLS
Main data file	MAIN	Yes	Yes	Yes	Yes
Recharge Package	RCH	Yes[1]	No	Yes	No
Well Package	WEL	Yes[1]	Yes	Yes	No
River Package	RIV	Yes[1]	Yes	Yes	No
Stream Package	STR	Yes[1]	Yes	Yes	No
Drain Package	DRN	Yes[1]	Yes	Yes	No
GHB Package	GHB	Yes[1]	Yes	Yes	No
ET Package	EVT	Yes[1]	No	Yes	No
Composite budget file	CBF	Transient only	Transient cross sections only	Optional[3]	No
Drawing commands file	DCF	No	User's option for mapview plots	Optional[3]	No
Endpoint file	ENDPOINT	Yes	Yes	Optional[3]	Endpoint mode
Pathline file	PATHLINE	Pathline mode	Pathline mode	Optional[3]	Pathline mode
Time series file	TIME-SERIES	Time-series mode	Time-series mode	Optional[3]	Time-series mode
Time data file	TIME	User's option	No	Optional[3]	No
Starting locations file	LOCATIONS	User's option	No	Optional[3]	No
Binary budget file	BUDGET	Yes[1]	No	Yes	Yes
Head file (ASCII text or binary)	HEAD HEAD(BINARY)	Yes[1]	Yes[2]	Yes	Yes[2]
Head format control file	HEAD-CONTROL	No	No	Optional[3]	User's option
Drawdown file (ASCII text or binary)	DRAWDOWN DRAWDOWN(BINARY)	No	User's option for mapview plots	Yes	User's option
Drawdown format control file	DRAWDOWN-CONTROL	No	No	Optional[3]	User's option
Contour data file	CONTOUR-DATA	No	User's option for mapview plots	Optional[3]	User's option
Contour format control file	CONTOUR-CONTROL	No	No	Optional[3]	User's option
Contour level file	CONTOUR-LEVEL	No	User's option for mapview plots	Optional[3]	No
Ancillary text data file	DATA	User's option	User's option	Yes	User's option
Summary output file	LIST	Yes	Yes	Optional[3]	No
Grid unit array file	GUA	No	User's option	Yes	No
Array data file (ASCII text or binary)	ARRAY ARRAY(BINARY)	No	No	Optional[3]	User's option
Array format control file	ARRAY-CONTROL	No	No	Optional[3]	User's option

Notes: 1. MODFLOW stress package, budget, and head files are not used by MODPATH in transient simulations that read data directly from a composite budget file.
2. The MODFLOW head file is not required by MODTOOLS or MODPATH-PLOT for some plot types.
3. Users have the option of specifying these files in the NAME file or allowing MODPATH to prompt for file names or, in some cases, assign default file names.

and format of the head data to be input and a file identified by the keyword DRAWDOWN-CONTROL for the drawdown values. MODTOOLS can use the files identified by the keywords ARRAY, ARRAY(BINARY), and ARRAY-CONTROL to create GIS output of cell values for miscellaneous gridded model data, such as hydraulic conductivity. MODTOOLS requires a file identified by the keyword ARRAY-CONTROL to determine the location and format of the miscellaneous gridded model data if these data are stored in a standard ASCII text file. The user should follow the instructions outlined in the MODFLOW manual for U2DREL (McDonald and Harbaugh, 1988, p. 14–4 to 14–5) for the format-control lines to create the files, CONTOUR-CONTROL, HEAD-CONTROL, DRAWDOWN-CONTROL, and ARRAY-CONTROL. Additional instructions are given in the "Format of Array Menu" section on p. 48.

Batch Use

When making a series of MODTOOLS runs using similar input and output options, the user can avoid having to answer the interactive menus every time by using the batch mode of MODTOOLS. MODTOOLS records the menu responses by the user to a file called **modtools.out** each time the MODTOOLS menu system is active. This file can be used as batch input in subsequent runs by renaming the file and specifying it on the command line. MODTOOLS operates in batch mode when the user specifies a batch file in the argument list input to the MODTOOLS AML program. The batch file consists of a fixed set of lines, which represents the user responses to the MODTOOLS menus. Each line is a response to one menu. The user can edit a line to change the operation of MODTOOLS and, thus, the resulting GIS output. For example, the user may wish to reduce the contour interval of a GIS output showing the lines of equal hydraulic head output by MODFLOW. Generally, simple changes are easily performed by most users while more caution is required for major changes. Batch files for each of the eight examples are listed in Appendix B.

Coordinate Systems

Mapviews

GIS output created by MODTOOLS must be referenced to real-world coordinates. MODTOOLS requires the user to specify coordinate information in order to translate particle coordinates from MODPATH into the coordinate system used in the user's GIS system. MODTOOLS prompts the user for unit-conversion multipliers, the origin of the MODFLOW grid, and a grid rotation angle to properly translate the particle coordinates for GIS output in mapview.

The unit-conversion multipliers are used to convert the units of length used in MODFLOW/ MODPATH to the proper units of length in the GIS coordinate system. MODTOOLS has two unit-conversion multipliers the x-y multiplier and z multiplier. The x-y multiplier is used to convert the units of length of x-y dimension. For example, if the model-grid dimensions are specified in MODFLOW or MODPATH using units of feet and the GIS output was required to have units of meters (to be compatible with other GIS data), the user would specify a multiplier of 0.3048 to convert feet to meters. The z

multiplier is used to convert the units of length of z dimension. For example, if the gridded model data output by MODFLOW were in units of feet and the GIS output was required to have units of meters (to be compatible with other GIS data), the user would specify a multiplier of 0.3048 to convert feet to meters.

The values for the x and y coordinates of the origin are used to properly translate the origin of the MODFLOW/MODPATH grid to the real-world coordinates in the desired coordinate system. These values represent the origin of the MODFLOW grid, which is the intersection of outer boundaries of the cell in row 1 and column 1 (upper left corner). The grid rotation angle is the angle in degrees that the model grid is rotated from north. The angle is specified in the counterclockwise degrees of rotation around the origin of the grid.

Vertical Profile Views

MODTOOLS can create vertical profile views along a row or column or along a particle pathline computed by MODPATH. To properly scale the GIS output from MODTOOLS, the user must specify a vertical exaggeration and a horizontal scale in addition to specifying the x-y and z unit-conversion multipliers. For example, if MODFLOW or MODPATH was operated using meters as the unit of length, MODTOOLS must convert the particle coordinates output by MODPATH as well as the cell geometry to units in feet to properly scale GIS output. The user would specify a multiplier of 0.3048 for the x-y and z unit-conversion multipliers to convert meters to feet.

For vertical profile views of contour GIS output, MODTOOLS constructs the GIS outputs and the accompanying model-grid GIS outputs using a "normalized" approach (Pollock, 1994, p. 4–12). MODTOOLS constructs a rectangular cross section using the average thickness of each layer. This approach is used for contour GIS output, because MODTOOLS uses the computer program CONTOUR (Harbaugh, 1990), which was designed to work with gridded data in mapview. CONTOUR has been adapted to work for vertical profile views, but the "normalized" approach must be used because of the numerical problems caused by vertical discretization schemes.

For vertical profile views of the other seven types of GIS output, MODTOOLS constructs a rectangular cross section of the cells using the input model-grid dimensions. This type of plot gives a better representation of grids with variable thickness layers.

Error Messages

Some error checking and prevention is done by the MODTOOLS program. MODTOOLS checks the list of arguments for several conditions; errors are reported to the user. MODTOOLS creates a file called MODTOOLS.LIST and several temporary data files that can be referred to if MODTOOLS fails to construct GIS output properly.

MODTOOLS records a listing of operations used to construct GIS output in the MODTOOLS.LIST file. MODTOOLS records these operations together with error messages, which are helpful to the user in resolving errors in the event MODTOOLS fails. MODTOOLS records operations starting with the process of reading the NAME file and ending with the construction of GIS output. Typically, errors encountered in reading the NAME file are caused by using FORTRAN unit numbers reserved for use by MODTOOLS (units 80–99) or improper keywords in the NAME file. A common error when constructing contour GIS output is not including the file containing the cell-by-cell terms in the MODTOOLS NAME file. This file is identified by the keyword CONTOUR-DATA in the NAME file. Another common error is not including the file containing the simulated head terms in the NAME file. MODTOOLS uses the head terms in vertical profile views for the tops of cells in layer 1 if layer 1 was simulated as a water-table layer. This file is identified by the keywords HEAD or HEAD(BINARY) in the MODTOOLS NAME file.

MODTOOLS records other useful information in the MODTOOLS.LIST file, such as the number of particles used to construct particle pathline GIS output and the number of cells omitted from a model-grid GIS output. Sometimes MODTOOLS must omit cells or particle pathlines because the polygons or lines cannot be represented properly in the GIS output when these features are projected onto the plane of view specified by the user. MODTOOLS records the number of dry cells omitted from the cell geometry and the number particles found in a user-specified time of travel in the MODTOOLS.LIST file. The user can review this file and check to see if any cells or particle pathlines were rejected.

MODTOOLS Menus

MODTOOLS uses an interactive menu and response system to obtain data from the user that controls the operations of MODTOOLS and the creation of the resulting GIS output. MODTOOLS menus are summarized in tables 3 and 4, which relate the GIS output to the specific menus. Only the appropriate menus for the selected GIS output are used in a MODTOOLS session. The choices available in each menu are discussed in the following sections. Most menus have a help option, which when selected, activates a help menu and message system. Most menus also have a "back" option, which enables the user to return to the previously seen menu and to reenter a response. Menu responses may be in either upper or lower case.

Table 3. MODTOOLS menus used to produce MODPATH GIS output

[X, menu is activated]

Menus	Particle pathlines			Particle endpoints	Particle time-series			Zones of transport		Model grid		
	View orientation			View orientation	View orientation			View orientation		View orientation		
	Map	Row/column	Particle path	Map	Map	Row/column	Particle path	Map	Row/column	Map	Row/column	Particle path
MODTOOLS options	X	X	X	X	X	X	X	X	X	X	X	X
Tracking mode				X								
Orientation	X	X	X	X	X	X	X	X	X	X	X	X
X-Y coordinate conversion	X	X	X	X	X	X	X	X	X	X	X	X
Z coordinate conversion	X	X	X	X	X	X	X	X	X	X	X	X
Rotation angle	X			X	X			X		X		
X origin	X			X	X			X		X		
Y origin	X			X	X			X		X		
Vertical exaggeration		X	X			X	X		X		X	X
Horizontal scale		X	X			X	X		X		X	X
Row, column, layer, ibound, or particle path selection		X	X			X	X		X		X	X
Equal sectors								X	X			

Table 4. MODTOOLS menus used to produce MODFLOW GIS output

[X, menu is activated]

Menus	Contours of Input and Output Arrays — View orientation				Velocity vectors — View orientation				Cell Values					
	Mapview layer	Row/column	Mapview ibound	Mapview upper	Mapview layer	Row/column	Mapview ibound	Mapview upper	Map	Mapview layer	Row/column	Particle path	Mapview ibound	Mapview upper
MODTOOLS options	X	X	X	X	X	X	X	X	X	X	X	X	X	X
MODFLOW package									X	X	X	X	X	X
Orientation	X	X	X	X	X	X	X	X	X	X	X	X	X	X
X-Y coordinate conversion	X	X[1]	X	X	X	X[1]	X	X			X[1]	X[1]		
Z coordinate conversion	X	X[1]	X	X	X	X[1]	X	X			X[1]	X[1]		
Rotation angle	X		X	X	X		X	X						
X origin	X		X	X	X		X	X						
Y origin	X		X	X	X		X	X						
Vertical exaggeration		X[1]				X[1]					X[1]	X[1]		
Horizontal scale		X[1]				X[1]					X[1]	X[1]		
Row, column, layer, ibound, or particle path selection	X	X	X	X	X	X	X	X	X	X	X		X	X
Format of array	X	X	X	X					X	X	X	X	X	X
Contour interval	X	X	X	X										
Scaling factor					X	X	X	X						
MODFLOW stress period	X	X	X	X					X	X	X	X	X	X
MODFLOW time step	X	X	X	X					X	X	X	X	X	X

Note: 1. Responses to these menus are applied to model-grid GIS output that accompanies this option.

Options Menu

The MODTOOLS Options menu (shown below) is the first menu displayed. The user determines the type of GIS output by selecting from one of eight choices. The first four choices produce GIS output using particle data output by MODPATH. The fifth choice produces a view of the model grid using data input to MODPATH. The last three choices produce GIS output using data arrays of MODFLOW. Data from a previous particle-tracking analysis using MODPATH is needed only for the first four choices.

```
Select an option for creating a coverage or info file(s)
-----------------------------------------------------------------
<cr> = Quit
   p = Pathline output
   e = Endpoint output
   t = Times-series output
   z = Zones-of-transport output
   g = Model-grid output
   c = Contour output
   v = Velocity-vector output
   i = Cell-value output
   h = Help

   Enter option:
```

Each option is summarized below:

   ----> p (Pathline output)

MODTOOLS constructs a pathline GIS output using the particle data recorded in the

PATHLINE file previously output by MODPATH. A particle pathline GIS output consists of a set of

connected lines for each particle. MODTOOLS appends to each line up to 62 characteristics associated

with each particle (see example 1 in Appendix B).

   ----> e (Endpoint output)

MODTOOLS constructs an endpoint GIS output using the particle data recorded in the

ENDPOINT file previously output by MODPATH. An endpoint GIS output consists of the starting or

final points, one for each particle. MODTOOLS appends to each point up to 32 characteristics associated

with each particle (see example 2 in Appendix B).

   ----> t (Time-series output)

MODTOOLS constructs a time-series GIS output using the particle data recorded in the

TIMESERS file previously output by MODPATH. A time-series GIS output consists of a set of points

for each particle at specified times of travel. MODTOOLS appends to each point up to 62 characteristics

associated with each particle (see example 3 in Appendix B).

----> z (Zones-of-transport output)

MODTOOLS constructs a zone-of-transport GIS output using the particle data recorded in the TIMESERS and ENDPOINT files previously output by MODPATH. MODPATH records particle data for each time of travel specified by the user in the TIMESERS file and the starting and final locations of the particles in the ENDPOINT file. MODTOOLS combines particle data recorded in both files and constructs two types of GIS output for this option. The first GIS output is the zones of transport, which consist of a set of polygons, one or more for each specified time of travel. MODTOOLS appends to each polygon the characteristic associated with the time of travel, which is represented by a model time step of MODPATH. The second GIS output consists of a set of points that form the vertices of each polygon; MODTOOLS appends to each vertex 33 characteristics associated with the particle that was used to determine each vertex (see example 4 in Appendix B).

----> g (Model-grid output)

MODTOOLS constructs model-grid GIS output using the data arrays defining grid dimensions from the MODPATH MAIN file. The model-grid GIS output consists of a set of polygons, one for each active cell. MODTOOLS appends to each polygon up to eight characteristics associated with each cell. The user need only assemble the MAIN file for mapview and for vertical profile views along a model row or column. The user will need to have previously completed a particle pathline analysis for GIS output of model-cell geometry along a particle pathline in the vertical profile view (see example 5 in Appendix B).

----> c (Contour output)

MODTOOLS constructs a contour GIS output using the cell-by-cell terms output by or input to MODFLOW or miscellaneous gridded model data. A contour GIS output consists of a set of contour lines connecting points of equal value, and MODTOOLS appends the value to each line. For a GIS output in mapview, MODTOOLS constructs only one GIS output, which consists of a set of lines connecting

points of equal value (see example 6 in Appendix B). For a GIS output in vertical profile view,

MODTOOLS also constructs a model-grid GIS output.

----> v (Velocity-vector output)

MODTOOLS constructs a velocity-vector GIS output using the cell-by-cell terms output by the

Basic and Block Centered Flow Packages of MODFLOW. A velocity-vector GIS output consists of one

line in each active cell that indicates the direction and magnitude of ground-water flow. MODTOOLS

appends eight characteristics to each vector. For a GIS output in mapview, MODTOOLS constructs only

one GIS output (see example 7 in Appendix B). For a GIS output in a vertical profile view, MODTOOLS

also constructs a model-grid GIS output.

----> i (Cell value output)

MODTOOLS constructs a cell-value GIS output using the data arrays output by or input to

MODFLOW. A cell-value GIS output consists of up to three GIS files, which contain one record for each

cell. A record consists of a set of characteristics associated with each cell. The number of characteristics

is dependent on the type of cell-by-cell terms selected, the number of layers in the model grid, and the

type of orientation (see example 8 in Appendix B).

Tracking Mode Menu

The MODPATH tracking menu is displayed only when the user specifies an endpoint GIS output.
The choice depends on the tracking mode (forward or backward) used in MODPATH during a particle-
tracking analysis. Endpoint GIS output is only available for mapview. This menu is used to select which
particle coordinates (starting locations or final locations) to use when constructing the endpoint GIS
output.


```
Select an option for creating a point coverage of starting or final locations
------------------------------------------------------------------
<cr> = Quit
   s = Mapview of starting locations (forward tracking)
   f = Mapview of final locations (forward tracking)
   e = Mapview of final locations (backward tracking)
   h = Help
   b = Back to MODTOOLS Options menu

   Enter tracking option:
```

Each option is summarized below:

----> s (starting locations, forward tracking)

MODTOOLS constructs an endpoint GIS output in mapview using the starting locations of the particles from a forward-tracking MODPATH simulation.

----> f (final locations, forward tracking)

MODTOOLS constructs an endpoint GIS output in mapview using the final locations of the particles from a MODPATH forward-tracking simulation.

----> e (final locations, backward tracking)

MODTOOLS constructs the endpoint GIS output in mapview using the final locations of the particles from a MODPATH backward-tracking simulation.

MODFLOW Package Menu

The MODFLOW package menu is displayed when the user specifies a cell-value GIS output. The user determines which cell-by-cell terms output by MODFLOW will be used to construct GIS output. MODTOOLS constructs GIS files when the user specifies a mapview orientation. MODTOOLS constructs three GIS files for the Block Centered Flow Package, one for each of the three principal directions of flow. MODTOOLS constructs one GIS file for each of the other MODFLOW packages. Model-grid GIS output is constructed when the user specifies a vertical profile orientation. The value of the cell-by-cell terms are appended to the set of characteristics for each cell of the model-grid GIS output in profile orientation.

```
Select the cell-by-cell terms from MODFLOW
-------------------------------------------------------------
<cr> = Quit
 hed = Head terms from Basic Package
 ddn = Drawdown terms from Basic Package
 bcf = Flow terms through cell faces from Block Centered Flow Package
 sto = Storage terms from Block Centered Flow Package
 riv = Flow terms from River Package
 rch = Flow terms from Recharge Package
 wel = Flow terms from Well Package
 drn = Flow terms from Drain Package
 ghb = Flow terms from General Head Boundary Package
 evt = Flow terms from Evapotranspiration Package
 str = Flow terms from Streamflow-Routing Package
 flo = Streamflow terms from Streamflow-Routing Package [flow]
 ibs = Storage terms from Interbed-Storage Package
 arr = Data array gridded like MODFLOW arrays
   h = Help
   b = Return to MODTOOLS Options menu

   Enter cell-by-cell term selection:
```

Each option is summarized below:

----> hed (head terms from Basic Package)

MODTOOLS constructs GIS output using the head values output by the Basic Package of MODFLOW. MODTOOLS will identify the file containing the terms using the keywords HEAD or HEAD(BINARY) in the NAME file. If the keyword HEAD is used in the NAME file, MODTOOLS needs another file identified by the keywords HEAD-CONTROL. The HEAD-CONTROL file contains format-control records used to read the head values. Instructions for creating the HEAD-CONTROL file are presented in the MODFLOW manual for U2DREL (McDonald and Harbaugh, 1988, p. 14–4 to 14–5).

----> ddn (drawdown terms from Basic Package)

MODTOOLS constructs GIS output using the drawdown values output by the Basic Package of MODFLOW. MODTOOLS will identify the file containing the terms using the keywords DRAWDOWN or DRAWDOWN(BINARY) in the NAME file. If the keyword DRAWDOWN is used in the NAME file, MODTOOLS needs another file identified by the keywords DRAWDOWN-CONTROL. The DRAWDOWN-CONTROL file contains format-control records used to read the drawdown values. Instructions for creating the DRAWDOWN-CONTROL file are presented in the MODFLOW manual for U2DREL (McDonald and Harbaugh, 1988, p. 14–4 to 14–5).

----> bcf (flow terms through cell faces from Block Centered Flow Package)

MODTOOLS constructs GIS output using the cell-by-cell terms output by the Block Centered Flow Package of MODFLOW. MODTOOLS can construct up to three GIS files depending on the orientation selected. MODTOOLS uses the flow terms through the right, front, and lower faces of a cell. MODTOOLS will identify the file containing the terms using the keywords BUDGET in the NAME file.

----> sto (storage terms from Block Centered Flow Package)

MODTOOLS constructs GIS output using the cell-by-cell storage output by the Block Centered Flow Package of MODFLOW. MODTOOLS will identify the file containing the terms using the keywords BUDGET in the NAME file.

----> riv, rch, wel, drn, ghb, evt, str, or ibs (select one only for other packages)

MODTOOLS constructs GIS output using the cell-by-cell flow terms output by the remaining packages of MODFLOW. MODTOOLS will identify the file containing the terms using the keywords BUDGET in the NAME file.

----> flo (streamflow terms from Streamflow-Routing Package)

MODTOOLS constructs GIS output using the streamflow terms output by the Streamflow-Routing Package (STR) developed by Prudic (1989) for MODFLOW. These terms are the cumulative streamflow for all streams occurring in each cell. MODTOOLS will identify the file containing the terms using the keywords BUDGET in the NAME file.

----> arr (data array gridded like MODFLOW arrays)

MODTOOLS constructs GIS output using miscellaneous gridded model data that are in the binary (unformatted) or standard ASCII text formats like those of MODFLOW. For example, MODTOOLS could construct a contour GIS output from the porosity array that was input to MODPATH. MODTOOLS will identify the file containing these miscellaneous data using the keywords ARRAY or ARRAY(BINARY) in the NAME file. In addition, MODTOOLS requires a file identified by the keyword, ARRAY-CONTROL, to determine the location and format of these data to be input. The ARRAY-CONTROL file contains format-control records, which MODTOOLS uses to operate the MODFLOW utility module U2DREL (McDonald and Harbaugh, 1988, p. 14–4 to 14–5) or an adapted U3DREL utility module from the MMSP programs (Scott, 1990, p. 197).

MODTOOLS will invoke the proper utility module using the user's response to the format of array menu. For MODTOOLS to read a data array in a binary format like those of MODFLOW, the format of the file containing this data array must match the binary format used by the array writing utility modules of MODFLOW. For MODTOOLS to read a data array in a ASCII text format like those of MODFLOW, the format of the file containing this data array must be readable by either the utility reading modules U2DREL of MODFLOW or U3DREL of MODTOOLS.

Orientation Menu

The orientation menu determines the type of view for all types of GIS output, except for an endpoint GIS output, which is available only in mapview. The choice of view orientation controls many of the subsequent menus. All eight possible choices are shown below; however, only the applicable choices appropriate for the type of GIS output request will be displayed during execution of MODTOOLS.

```
Select an orientation for the MODTOOLS GIS output
------------------------------------------------------------------
<cr> = Quit
  m = Mapview
  m = Mapview, characteristics for all layers will be generated
  l = Mapview of a user-specified model layer
  i = Mapview of a user-specified model ibound value
  u = Mapview of uppermost active cells
  r = Vertical profile view along a row
  c = Vertical profile view along a column
  p = Vertical profile view along a user-specified particle path
  h = Help
  b = Back to MODTOOLS Options menu

  Select an orientation:
```

Each option is summarized below:

> **----> m (Mapview)**

The specified GIS output is constructed in mapview (the x-y plane of the model grid).

> **----> m (Mapview, characteristics for all layers will be generated)**

MODTOOLS displays this option only when the user specifies cell-value GIS output from the cell-by-cell terms of MODFLOW. This option is useful for translating the cell-by-cell terms of MODFLOW into a GIS format. MODTOOLS constructs up to three GIS files depending on which cell-by-cell term output by a MODFLOW package was selected from the MODFLOW package menu.

> **----> l (Mapview of a user-specified model layer)**

MODTOOLS displays this option only when the user specifies contour, velocity-vector, or cell-value GIS outputs. MODTOOLS constructs the GIS output for cells in a user-specified layer.

> **----> i (Mapview of a user-specified model ibound value)**

MODTOOLS displays this option only when the user specifies contour, velocity-vector, or cell-value GIS outputs. MODTOOLS constructs the GIS output for cells that are identified by a value assigned in the IBOUND array. Commonly, an aquifer will be simulated by more than one layer in a ground-water model using MODFLOW, such as in the sample problems developed by Pollock (1994). The user can set the values that were assigned to each cell in the IBOUND array to reflect this vertical discretization scheme.

f----> u (Mapview of uppermost active cells)

This option applies only when the user specifies that MODTOOLS construct contour, velocity-vector, or cell-value GIS outputs. MODTOOLS constructs the GIS output for the uppermost active cells. This option is useful for constructing GIS output from ground-water models which simulate a water table in cells other than in layer 1 of the model grid. MODTOOLS omits cells from the specified GIS output under several conditions. MODTOOLS automatically omits inactive cells (cell IBOUND=0). MODTOOLS omits cells that have a value of the cell-by-cell term equal to the user-specified head for dry cells (HDRY item in MAIN file) or no-flow cells (HNOFLO item in MAIN file).

----> r (vertical profile view along a row)

MODTOOLS constructs the specified GIS output in a vertical profile along a specified row.

----> c (vertical profile view along a column)

MODTOOLS constructs the specified GIS output in a vertical profile along a specified column.

----> p (vertical profile view along a user-specified particle path)

This option applies only when the user specifies that MODTOOLS construct a pathline, time-series, model-grid, or cell-value GIS output. MODTOOLS constructs the specified GIS output in a vertical profile view along a specified particle path.

X-Y Coordinate Conversion Menu

For mapview orientations, GIS output created by MODTOOLS must be referenced to real-world coordinates to allow proper display of the output. The x-y coordinate conversion multipliers are used to convert the units of length used in MODFLOW/MODPATH to the units of length in the desired coordinate system for the GIS.

For vertical orientations, MODTOOLS requires that particle and cell coordinates have units of length in feet to properly apply the vertical exaggeration and horizontal map scale. The user would specify option 2 in the menu to convert meters to feet if the units of length used in MODFLOW or MODPATH were in meters.

```
X,Y coordinate conversion
 Select option to convert from model units to GIS length units.
  (Note: For vertical profile orientations, MODTOOLS requires
  coordinates in units of feet).
---------------------------------------------------------------
<cr> = Quit
   0 = None
   1 = Feet to meters
   2 = Meters to feet
   User-specified multiplication factor
   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter option:
```

----> 0 (none)

This option causes MODTOOLS to keep particle or cell coordinates in the MODPATH coordinate system specified by the user.

----> 1 (feet to meters)

This option causes MODTOOLS to translate the particle or cell coordinates from units of feet to units of meters. MODTOOLS multiples the x and y coordinates by a factor of 0.3048.

----> 2 (meters to feet)

This option causes MODTOOLS to translate the particle or cell coordinates from units of meters to units of feet. MODTOOLS multiplies the x and y coordinates by a factor of 3.281.

----> User-specified multiplication factor

This option causes MODTOOLS to multiply the particle or cell coordinates by a factor specified by the user.

Z Coordinate Conversion Menu

The z coordinate conversion multiplier is used to convert the units of length in the vertical direction used in MODFLOW/MODPATH to the units of length in the desired coordinate system for the GIS. For example, if the simulated head output by MODFLOW were in units of feet and the user wanted to produce contours in units of meters, the user would specify option 1. For vertical orientations, MODTOOLS **requires** the particle and cell coordinates have units of length in feet to properly apply the vertical exaggeration and horizontal map scale. The user would specify option 2 in the menu to convert meters to feet if the units of length used in MODFLOW/MODPATH were in meters.

```
Z coordinate conversion
 Select option to convert from model units to GIS length units.
  (Note: For vertical profile orientations, MODTOOLS requires
  coordinates in units of feet).
-----------------------------------------------------------------
<cr> = Quit
   0 = None
   1 = Feet to meters
   2 = Meters to feet
   User-specified multiplication factor
   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter option:
```

----> 0 (none)

This option causes MODTOOLS to keep particle or cell coordinates in the MODPATH coordinate system specified by the user.

----> 1 (feet to meters)

This option causes MODTOOLS to translate the particle or cell coordinates from units of feet to units of meters. MODTOOLS multiplies the z coordinates by a factor of 0.3048.

----> 2 (meters to feet)

This option causes MODTOOLS to translate the particle or cell coordinates from units of meters to units of feet. MODTOOLS multiplies the z coordinates by a factor of 3.281.

----> User-specified multiplication factor

This option causes MODTOOLS to multiply the z coordinates of particle or cell by a factor specified by the user.

Rotation Angle Menu

MODTOOLS displays this menu only when the user specifies a mapview orientation for some GIS outputs. The rotation angle menu is activated by MODTOOLS to provide a means to rotate, in a counterclockwise direction, the x and y coordinates of particles and cells to align them with the orientation of the model grid in the real world. The step of rotating these coordinates is another step in translating particle or cell coordinates from the MODPATH coordinate system to the GIS coordinate system. The grid rotation angle is the angle in degrees that the MODFLOW grid has been rotated from north. The angle is specified in the counterclockwise degrees of rotation around the origin of the MODFLOW grid.

```
counterclockwise rotation angle around MODFLOW origin
-----------------------------------------------------------------------
<cr> = Quit
   0 = None
   User-specified rotation angle
   h = Help
   b = Back to MODTOOLS Orientation menu

  Enter counterclockwise rotation angle:
```

X-Origin Menu

MODTOOLS displays this menu only when the user specifies a mapview orientation. The x origin menu is activated by MODTOOLS to provide a means to translate the x and y components of the particle or cell coordinates from the MODPATH coordinate system to the GIS coordinate system. The user enters the x coordinate of the MODFLOW origin using the real-world coordinate. The origin of the MODFLOW grid is the intersection of outer boundaries of the cell in row 1 and column 1.

```
X-origin of MODFLOW grid
-----------------------------------------------------------------------
<cr> = Quit
   0 = None
   User-specified X-origin coordinate
   h = Help
   b = Back to MODTOOLS Orientation menu

  Enter x-origin:
```

Y-Origin Menu

MODTOOLS displays this menu only when the user specifies a mapview orientation. The y origin menu is activated by MODTOOLS to provide a means to translate the x and y components of the particle or cell coordinates from the MODPATH coordinate system to the GIS coordinate system. The user enters the y coordinate of the MODFLOW origin using the real-world coordinate. The origin of MODFLOW model grid is the intersection of outer boundaries of the cell in row 1 and column 1.

```
Y-origin of MODFLOW grid
-----------------------------------------------------------------------
<cr> = Quit
   0 = None
   User-specified Y-origin coordinate
   h = Help
   b = Back to MODTOOLS Orientation menu

  Enter y-origin:
```

Vertical Exaggeration Menu

MODTOOLS displays this menu only when the user specifies a vertical profile orientation. The vertical exaggeration menu is activated by MODTOOLS to provide a means to exaggerate the vertical

component of the particle or cell coordinates. The user enters any positive number. MODTOOLS uses this value as a multiplier to exaggerate the z coordinates of the GIS output in a vertical profile view.

```
Enter vertical exaggeration
---------------------------------------------------------------------
<cr> = Quit
    User-specified vertical exaggeration factor
    h = Help
    b = Back to MODTOOLS Orientation menu

Enter vertical exaggeration 1 foot = n feet:
```

Horizontal Scale Menu

MODTOOLS displays this menu only when the user specifies a vertical profile orientation. The horizontal map-scale menu is activated by MODTOOLS to provide a means to scale the horizontal component of the particle or cell coordinates of the GIS output in a vertical profile view. The user enters any positive number. For example, to create a view with a horizontal scale of 1:24,000, the user would enter 24000.

```
Enter horizontal mapscale
---------------------------------------------------------------------
<cr> = Quit
    User-specified horizontal mapscale
    h = Help
    b = Back to Vertical Exaggeration menu

Enter horizontal mapscale 1 foot = n feet:
```

Row, Column, Layer, Ibound, or Particle Path Menu

This menu is activated by MODTOOLS to provide a means to choose a row, column, or layer from the model grid, a cell IBOUND value, or a particle pathline. MODTOOLS uses this choice to construct GIS output along a specified row, column, or layer of the model grid, for model cells having specified IBOUND values, or along a specified particle pathline. The title of this menu is determined by the type of orientation of the GIS output specified by the user.

```
Enter number of model layer to view
---------------------------------------------------------------------
<cr> = Quit
    User-specified selection
    h = Help
    b = Back to MODTOOLS Orientation menu

  Enter selection:
```

Format of Array Menu

   This menu is activated by MODTOOLS to provide a means to specify the format of the gridded model data for constructing contour and cell-value GIS outputs. MODTOOLS uses this choice to determine how to read gridded model data of MODFLOW and MODPATH, and miscellaneous gridded model data, such as hydraulic conductivity. These data can be provided in a standard ASCII text file or in a binary (unformatted) file. MODTOOLS identifies the file containing these data using the keyword CONTOUR-DATA for contour GIS output, and HEAD or HEAD(BINARY), DRAWDOWN or DRAWDOWN(BINARY), BUDGET, and ARRAY or ARRAY(BINARY) for cell-value GIS output. MODTOOLS applies the user's choice and information in a file identified by the keyword, CONTOUR-CONTROL for contour GIS output or HEAD-CONTROL,DRAWDOWN-CONTROL, or ARRAY-CONTROL for cell-value GIS output, to determine the location and format of the data.

   MODTOOLS uses the utility reader U2DREL of MODFLOW to read data with a "two-dimensional array" format, such as the head and drawdown values recorded by MODFLOW. The user should follow the instructions outlined in the MODFLOW manual for the utility reader U2DREL (McDonald and Harbaugh, 1988, p. 14–4 to 14–5) to create the array-control files such as HEAD-CONTROL.

   MODTOOLS uses the utility reader U3DREL, which was adapted from the MMSP program (Scott, 1990, p. 197) to read data with a "three-dimensional array" format, such as the cell-by-cell flow terms from the Block Centered Flow Package recorded by MODFLOW. The user follows the instructions in the MODFLOW manual for the utility reader U2DREL (McDonald and Harbaugh, 1988, p. 14–4 to 14–5) to create the files, CONTOUR-CONTROL for contour GIS output, and ARRAY-CONTROL, for cell-value GIS output. However, the user needs to include only a single array-control record that is used to read the values for all layers.

```
Enter dimension of the gridded model data
----------------------------------------------------------------
<cr> = Quit
   2 = Two-dimensional array
   3 = Three-dimensional array
   b = Back to MODTOOLS Orientation menu
   h = Help

Enter dimension of gridded data:
```

    ----> 2

   This option causes MODTOOLS to read the gridded model data using the utility reader U2DREL of MODFLOW (McDonald and Harbaugh, 1988, p. 14–4 to 14–5).

    ----> 3

   This option causes MODTOOLS to read the gridded model data using a utility reader U3DREL adapted from the MMSP program (Scott, 1990, p. 197).

Contour Interval Menu

This menu is activated by MODTOOLS to provide a means to specify the contour interval that will be used by MODTOOLS to create the contour GIS output consisting of lines connecting points of equal value from the gridded model data.

```
Enter contour interval
-------------------------------------------------------------------
<cr> = Quit
   User-specified contour interval
   b = Back to MODTOOLS Orientation menu
   h = Help

Enter contour interval:
```

Scaling Factor Menu

MODTOOLS displays this menu only when the user specifies the option for velocity-vector GIS output. This menu is activated by MODTOOLS to provide a means to specify the scaling factor that will be used by MODTOOLS to create GIS output of lines showing the velocity vectors. MODTOOLS uses two procedures to create a line representing the magnitude of the velocity vector in each active cell of the model grid. A positive number causes MODTOOLS to use an arithmetic scaling procedure directly adapted from the programs developed by Scott (1990, p. 64). When arithmetic scaling is selected, the length of each velocity vector is multiplied by the user-specified scaling factor. A negative number causes MODTOOLS to use a logarithmic scaling procedure. When logarithmic scaling is selected, MODTOOLS computes the minimum power-of-10 multiplier needed to increase the minimum nonzero vector length to a value greater than one. The length of each velocity vector is computed by multiplying by the computed power-of-10, then taking the base-10 logarithm of the product, and finally multiplying by the absolute value of a user-specified scaling factor.

```
Enter scaling factor for length of velocity vector
-------------------------------------------------------------------
<cr> = Quit
   n > 0 - arithmetic scaling
   n = 0 - no scaling
   n < 0 - logarithmic scaling
   h = Help
   b = Back to MODTOOLS Orientation menu

Enter scaling factor, n:
```

MODFLOW Stress Period Menu

MODTOOLS displays this menu only when the user specifies the option for contour and cell-value GIS output. This menu provides a means for the user to specify the stress period to MODTOOLS. MODTOOLS uses this choice to select the proper stress period of the cell-by-cell terms output from a transient ground-water simulation. MODFLOW records cell-by-cell terms at a stress period specified by

the user in a transient ground-water simulation. MODTOOLS will omit all terms that do not have the proper stress period.

```
Enter MODFLOW stress period number for the cell-by-cell terms
--------------------------------------------------------------------
<cr> = Quit
   User-specified stress period
   h = Help
   b = Back to MODTOOLS Orientation menu


Enter stress period number:
```

MODFLOW Time Step Menu

　　　　MODTOOLS displays this menu only when the user specifies the option for contour and cell-value GIS output. This menu provides a means for the user to specify the time step to MODTOOLS. MODTOOLS uses this choice to select the proper time step of the cell-by-cell terms output from a transient ground-water simulation. MODTOOLS will omit all terms that do not have the proper time step for the stress period specified by the user.

```
Enter MODFLOW time step number for cell-by-cell terms
---------------------------------------------------------------------
<cr> = Quit
   User-specified time step
   h = Help
   b = Back to MODTOOLS Orientation menu

Enter time step number:
```

Equal Sectors Menu

　　　　MODTOOLS displays this menu only when the user specifies the option for zones of transport GIS output. This menu is activated by MODTOOLS to provide a means to specify the number of equal sectors used to compute the vertices of polygons that will represent the zones of transport. MODTOOLS uses this choice to compute polygons that represent the projection of the zones of transport to wells onto a user-specified plane of the model grid. The algorithm searches each sector to locate the particle that represents the maximum distance traveled from the center of the cell containing the well for the specified time of travel (see Appendix C for more information).

```
Enter number of equal sectors used to delineate zones of transport
---------------------------------------------------------------------
<cr> = Quit
   User-specified number of sectors
   h = Help
   b = Back to MODTOOLS Orientation menu

Enter number of equal sectors
```

Descriptions of GIS Output Files

MODTOOLS creates several different types of GIS output from particle data recorded by MODPATH during a particle-tracking analysis, from gridded data of MODFLOW, or from miscellaneous gridded model data. During the process of creating GIS output, MODTOOLS associates particle and cell characteristics recorded by MODPATH to the appropriate particle or cell in the GIS output. MODTOOLS also associates characteristics to contour lines and velocity vectors that are derived from gridded model data, such as head values or flow terms output by MODFLOW. The values of these characteristics are recorded by MODTOOLS in data terms of the GIS output, called attributes in GIS nomenclature. Each attribute must be defined in the GIS output by type (integer or real number), by the number of digits needed to store and display the value of the attribute (input and output width), and by the number of decimal places. The input and output width of some attributes that are associated with cell characteristics such as the row, column, or layer, are determined by MODTOOLS using the number of rows, columns, and layers defining the model grid.

Output from MODPATH

As part of the GIS output it constructs, MODTOOLS creates a set of attributes from each record of particle data output by MODPATH in the ENDPOINT, PATHLINE, and TIMESERS files. ENDPOINT, PATHLINE, and TIMESERS output from MODPATH all contain particle positions and characteristics in space and time. Several criteria determine whether MODPATH writes a record of data for each particle position (Pollock, 1994). Particle positions are recorded in both local and global coordinates. Local coordinates are relative within the boundaries of each cell, whereas global coordinates are relative to the entire model grid.

Particle characteristics contain information concerning the location, velocity, and travel time of individual particles during a particle-tracking analysis. Each particle travels from a start position to a final position. Intermediate positions and characteristics along this pathline are recorded when a particle intercepts a cell boundary and at user-specified times (Pollock, 1994). A single particle may travel along a pathline that is described by a set of positions: a start position (point 1 in fig. 11), intermediate positions (points 2 and 3 in fig. 11), and a final position (point 4 in fig. 11). The segment of the pathline connecting particle positions is termed an "arc" in GIS nomenclature. Each particle position and characteristics associated with this position within the model grid are output by MODPATH as a record of data in one or more output files. The positions shown in figure 11 would be represented by four records of particle data output by MODPATH in the PATHLINE file. These positions would be represented by one record in the ENDPOINT file and up to four records in the TIMESERS file (determined if the particle-tracking time equaled the user-specified times).

The starting position is the initial position of a particle at the beginning of a simulation. Characteristics that are derived from this position are termed "start attributes." The names of these attributes in GIS files are prefixed with the character string STR. Particle characteristics describing row, column, and layer positions and local and global x and y coordinates within the model cell and model

Locations where attribute values are evaluated:

Start attributes:	Arc A	Arc B	Arc C
STRSTP	at 1	at 1	at 1
STRTIM	at 1	at 1	at 1
STRCOL	at 1	at 1	at 1
STRROW	at 1	at 1	at 1
STRLAY	at 1	at 1	at 1
STRIBD	at 1	at 1	at 1
STRXGC	at 1	at 1	at 1
STRXLC	at 1	at 1	at 1
STRYGC	at 1	at 1	at 1
STRYLC	at 1	at 1	at 1
STRZGC	at 1	at 1	at 1
STRZLC	at 1	at 1	at 1

Last attributes:			
LSTTIM	at 1	at 2	at 3
LSTCOL	at 1	at 2	at 3
LSTROW	at 1	at 2	at 3
LSTLAY	at 1	at 2	at 3
LSTIBD	at 1	at 2	at 3
LSTXGC	at 1	at 2	at 3
LSTXLC	at 1	at 2	at 3
LSTYGC	at 1	at 2	at 3
LSTYLC	at 1	at 2	at 3
LSTZGC	at 1	at 2	at 3
LSTZLC	at 1	at 2	at 3

Present attributes:			
PRESTP	at 2	at 3	at 4
PRETIM	at 2	at 3	at 4
PRECOL	at 2	at 3	at 4
PREROW	at 2	at 3	at 4
PRELAY	at 2	at 3	at 4
PREIBD	at 2	at 3	at 4
PREXGC	at 2	at 3	at 4
PREXLC	at 2	at 3	at 4
PREYGC	at 2	at 3	at 4
PREYLC	at 2	at 3	at 4
PREZGC	at 2	at 3	at 4
PREZLC	at 2	at 3	at 4
PRETRV	1 to 2	2 to 3	3 to 4
PREXVL	1 to 2	2 to 3	3 to 4
PREYVL	1 to 2	2 to 3	3 to 4
PREZVL	1 to 2	2 to 3	3 to 4
PRESPD	1 to 2	2 to 3	3 to 4

Cumulative attributes:			
CUMXVL	1 to 2	1 to 3	1 to 4
CUMYVL	1 to 2	1 to 3	1 to 4
CUMZVL	1 to 2	1 to 3	1 to 4
CUMSPD	1 to 2	1 to 3	1 to 4

Final attributes:			
FINSTP	at 4	at 4	at 4
FINTIM	1 to 4	1 to 4	1 to 4
FINCOL	at 4	at 4	at 4
FINROW	at 4	at 4	at 4
FINLAY	at 4	at 4	at 4
FINIBD	at 4	at 4	at 4
FINZGC	at 4	at 4	at 4
FINXGC	at 4	at 4	at 4
FINXLC	at 4	at 4	at 4
FINYGC	at 4	at 4	at 4
FINYLC	at 4	at 4	at 4
FINZLC	at 4	at 4	at 4
FINXVL	1 to 4	1 to 4	1 to 4
FINYVL	1 to 4	1 to 4	1 to 4
FINZVL	1 to 4	1 to 4	1 to 4
FINSPD	1 to 4	1 to 4	1 to 4
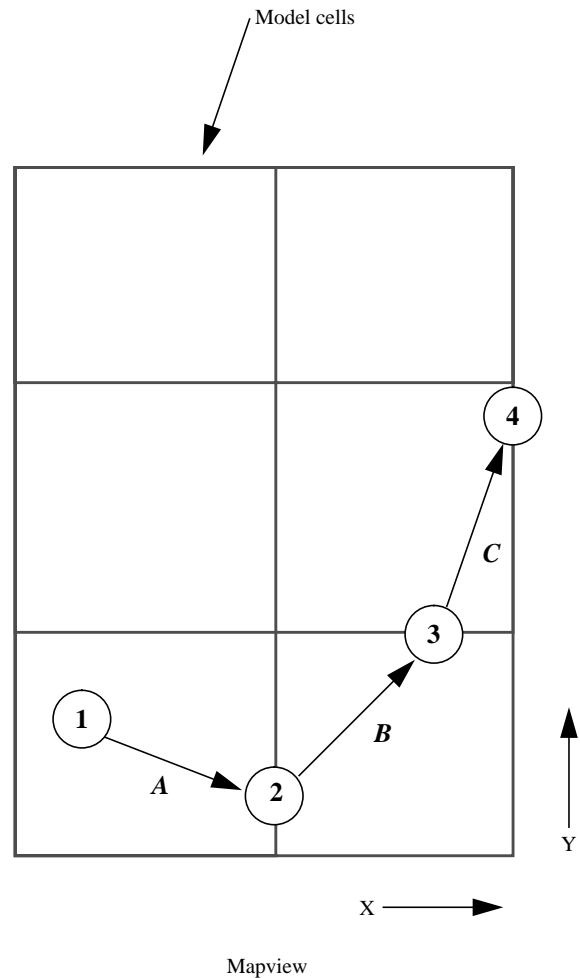
Figure 11. Example showing the backward movement of a particle and attributes created for the particle. (See tables 5 and 6 for descriptions of attributes).

grid, respectively, are recorded along with the vertical position of each particle within a cell (local z-elevation) and within the model grid (global z-elevation). MODTOOLS records this information for each particle and associates these attributes to the appropriate particle.

Intermediate positions that are occupied by particles during a simulation are described by last, present, and cumulative attributes. These attributes are evaluated for each arc of a pathline and may contain redundant information. Last attributes describe particle positions and characteristics at a previous position that is occupied by a particle during a simulation. Names of these attributes in GIS files are prefixed with the character string LST. Present attributes describe current particle positions and characteristics. Present attributes are evaluated along each arc using the previous position and the current position, which describe the arc. Names of these attributes in GIS files are prefixed with the character string PRE. Cumulative attributes describe particle positions and characteristics during a simulation using the start position and the current position. Cumulative attributes are evaluated along each arc. Names of these attributes in GIS files are prefixed with the character string CUM. This information is recorded for each particle. Final attributes are evaluated at the end of the pathline. Names of these attributes in GIS files are prefixed with the character string FIN. This information is recorded for each particle.

For this example, a single particle is tracked backward through cells to a recharge-source cell (fig. 11). Point 1 is assigned the start position information and this information is recorded. As this selected particle moves through other cells, last, present, and cumulative attributes for intermediate positions at points 2 and 3 are evaluated and recorded. At this point in the simulation, some information is identical for these attributes from arcs A and B. If more intermediate positions exist, these attributes would differ. At point 4, last, present, and cumulative attributes for arc C are again evaluated and recorded. At point 4, final attributes for this particle are evaluated and recorded for arcs A, B, and C. The method of assigning attributes to particles and arcs is identical for forward-tracked particles.

Pathline and Time-Series Data

MODTOOLS constructs pathline and time-series GIS output from particle data recorded in the PATHLINE and TIMESERS files. MODTOOLS computes 62 characteristics associated with each particle position (table 5). The pathline GIS output has line topology and consists of a series of connected lines for each particle pathline. Attributes derived from particle characteristics in the PATHLINE output by MODPATH are assigned to each line. A time-series GIS output has point topology and consists of a set of points at specified times of travel along each pathline. In this case, the attributes are assigned to each point.

Table 5. Attributes associated with pathline and time-series GIS output from MODTOOLS

[n, width determined by MODTOOLS from model grid]

Attribute name	Item type	Input width	Output width	Number of decimals	Description
PARTID	Integer	10	10	0	Particle-id from PATHLINE or TIMESERS files output by MODPATH
STRSTP	Integer	10	10	0	Starting time step
STRTIM	Floating	16	8	3	Starting time of particle at time zero
STRROW	Integer	n	n	0	Starting row at time STRTIM
STRCOL	Integer	n	n	0	Starting column at time STRTIM
STRLAY	Integer	n	n	0	Starting model layer at time STRTIM
STRIBD	Integer	10	10	0	Starting model ibound value at time STRTIM
STRXGC	Floating	8	16	3	Starting global particle x-coordinate at time STRTIM
STRXLC	Floating	8	16	3	Starting local particle x-coordinate at time STRTIM
STRYGC	Floating	8	16	3	Starting global particle y-coordinate at time STRTIM
STRYLC	Floating	8	16	3	Starting local particle y-coordinate at time STRTIM
STRZGC	Floating	8	16	3	Starting global particle z-coordinate at time STRTIM
STRZLC	Floating	8	16	3	Starting local particle z-coordinate at time STRTIM
FINSTP	Integer	10	10	0	Final time step
FINTIM	Floating	8	16	3	Final cumulative time of particle
FINROW	Integer	n	n	0	Final row at time FINTIM
FINCOL	Integer	n	n	0	Final column at time FINTIM
FINLAY	Integer	n	n	0	Final model layer at time FINTIM
FINIBD	Integer	10	10	0	Final model ibound value at time FINTIM
FINXGC	Floating	8	16	3	Final global particle x-coordinate at time FINTIM
FINXLC	Floating	8	16	3	Final local particle x-coordinate at time FINTIM
FINYGC	Floating	8	16	3	Final global particle y-coordinate at time FINTIM
FINYLC	Floating	8	16	3	Final local particle y-coordinate at time FINTIM
FINZGC	Floating	8	16	3	Final global particle z-coordinate at time FINTIM
FINZLC	Floating	8	16	3	Final local particle z-coordinate at time FINTIM
FINXVL	Floating	8	16	8	Particle x-direction velocity along entire particle path
FINYVL	Floating	8	16	8	Particle y-direction velocity along entire particle path
FINZVL	Floating	8	16	8	Particle z-direction velocity along entire particle path
FINSPD	Floating	8	16	8	Particle speed along entire particle path
LSTTIM	Floating	8	16	3	Last time of particle
LSTROW	Integer	n	n	0	Last row at time LSTTIM
LSTCOL	Integer	n	n	0	Last column at time LSTTIM
LSTLAY	Integer	n	n	0	Last model layer at time LSTTIM

Table 5. Attributes associated with pathline and time-series GIS output from MODTOOLS—Continued

[n, width determined by MODTOOLS from model grid]

Attribute name	Item type	Input width	Output width	Number of decimals	Description
LSTIBD	Integer	10	10	0	Last model ibound value at time LSTTIM
LSTXGC	Floating	8	16	3	Last global particle x-coordinate at time LSTTIM
LSTXLC	Floating	8	16	3	Last local particle x-coordinate at time LSTTIM
LSTYGC	Floating	8	16	3	Last global particle y-coordinate at time LSTTIM
LSTYLC	Floating	8	16	3	Last local particle y-coordinate at time LSTTIM
LSTZGC	Floating	8	16	3	Last global particle z-coordinate at time LSTTIM
LSTZLC	Floating	8	16	3	Last local particle z-coordinate at time LSTTIM
PRESTP	Integer	10	10	0	Present time step
PRETIM	Floating	8	16	3	Present time of particle
PREROW	Integer	n	n	0	Present row at time PRETIM
PRECOL	Integer	n	n	0	Present column at time PRETIM
PRELAY	Integer	n	n	0	Present model layer at time PRETIM
PREIBD	Integer	10	10	0	Present model ibound value at time PRETIM
PREXGC	Floating	8	16	3	Present global particle x-coordinate at time PRETIM
PREXLC	Floating	8	16	3	Present local particle x-coordinate at time PRETIM
PREYGC	Floating	8	16	3	Present global particle y-coordinate at time PRETIM
PREYLC	Floating	8	16	3	Present local particle y-coordinate at time PRETIM
PREZGC	Floating	8	16	3	Present global particle z-coordinate at time PRETIM
PREZLC	Floating	8	16	3	Present local particle z-coordinate at time PRETIM
PRETRV	Floating	8	16	3	Travel time along this arc
PREXVL	Floating	8	16	8	Present particle x-direction velocity along pathline
PREYVL	Floating	8	16	8	Present particle y-direction velocity along pathline
PREZVL	Floating	8	16	8	Present particle z-direction velocity along pathline
PRESPD	Floating	8	16	8	Present particle speed along pathline
CUMXVL	Floating	8	16	8	Cumulative particle x-direction velocity along particle path from start to present
CUMYVL	Floating	8	16	8	Cumulative particle y-direction velocity along particle path from start to present
CUMZVL	Floating	8	16	8	Cumulative particle z-direction velocity along particle path from start to present
CUMSPD	Floating	8	16	8	Cumulative particle speed along particle path from start to present
MODSTP	Integer	10	10	0	Cumulative MODFLOW time step number (Pollock, 1994, p. B–4)

Endpoint Data

MODTOOLS constructs endpoint GIS output from particle data recorded in the ENDPOINT file. MODTOOLS computes 32 attributes associated with each particle position (table 6). Intermediate attributes like those from the pathline and time-series GIS outputs are not present because intermediate particle positions are not recorded in the ENDPOINT file by MODPATH.

Zones of Transport Data

MODTOOLS constructs zones of transport GIS output from particle data recorded in the TIMESERS and ENDPOINT files of a backward-tracking analysis. MODTOOLS constructs two types of GIS output from the combined particle data. The first consists of polygons that represent the projection of the zones of transport onto the user-specified plane of the model grid. Only one attribute, TIMSTP, is associated with each polygon (table 7). This attribute identifies the model time step associated with each polygon that represents a zone of transport.

The second GIS output constructed by MODTOOLS for the zones of transport GIS output has "point topology," which means this GIS output consists of points that represent the vertices of the zones of transport polygons. The attributes associated with these vertices are derived from particle characteristics of the particle used to derive the vertices, as described in Appendix C.

Model Grid

MODTOOLS constructs GIS output of model-cell geometry using the cell data recorded in the MAIN file. The MAIN file contains information about the cell spacing in the model grid as well as data about whether a cell is active or inactive. MODTOOLS can construct two types of GIS output, which show different views of the model grid, mapview and vertical profile. The number of attributes associated with each cell (polygon) is determined by the view. All possible attributes are listed in table 8. Vertical profile views may be along a model row or column, or a user-specified particle path. Eight attributes, shown in table 8, are computed by MODTOOLS for vertical profile GIS output. For mapview GIS output of the model grid, the last four attributes shown in table 8, IBOUND, TOPELEV, BOTELEV, and THICK, are not included in the attributes. MODTOOLS constructs "normalized" cross sections (like those constructed by MODPATH-PLOT (Pollock, 1994, p. 4–12) to accompany contour and velocity-vector GIS output created using vertical profile orientations. MODTOOLS computes an average thickness for each model layer and generates a rectangular cross section with layers of constant thickness. To accompany the remaining six types of GIS output created using vertical profile orientations, MODTOOLS uses the top and bottom elevations of the cells read from the MAIN file to construct a cross section. Each cell is constructed as a rectangle, which allows the shape of variable thickness and dipping layers to be viewed.

Table 6. Attributes associated with endpoint GIS output from MODTOOLS

[n, width determined by MODTOOLS from model grid]

Attribute name	Item type	Input width	Output width	Number of decimals	Description
PARTID	Binary	4	5	0	Particle-id from ENDPOINT files output by MODPATH
STRTIM	Floating	8	16	3	Starting time of particle at time zero
STRROW	Integer	n	n	0	Starting row at time STRTIM
STRCOL	Integer	n	n	0	Starting column at time STRTIM
STRLAY	Integer	n	n	0	Starting model layer at time STRTIM
STRIBD	Integer	10	10	0	Starting model ibound value at time STRTIM
STRXGC	Floating	8	16	3	Starting global particle x-coordinate at time STRTIM
STRXLC	Floating	8	16	3	Starting local particle x-coordinate at time STRTIM
STRYGC	Floating	8	16	3	Starting global particle y-coordinate at time STRTIM
STRYLC	Floating	8	16	3	Starting local particle y-coordinate at time STRTIM
STRZGC	Floating	8	16	3	Starting global particle z-coordinate at time STRTIM
STRZLC	Floating	8	16	3	Starting local particle z-coordinate at time STRTIM
FINTIM	Floating	8	16	3	Final cumulative time of particle
FINROW	Integer	n	n	0	Final row at time FINTIM
FINCOL	Integer	n	n	0	Final column at time FINTIM
FINLAY	Integer	n	n	0	Final model layer at time FINTIM
FINIBD	Integer	10	10	0	Final model ibound value at time FINTIM
FINXGC	Floating	8	16	3	Final global particle x-coordinate at time FINTIM
FINXLC	Floating	8	16	3	Final local particle x-coordinate at time FINTIM
FINYGC	Floating	8	16	3	Final global particle y-coordinate at time FINTIM
FINYLC	Floating	8	16	3	Final local particle y-coordinate at time FINTIM
FINZGC	Floating	8	16	3	Final global particle z-coordinate at time FINTIM
FINZLC	Floating	8	16	3	Final local particle z-coordinate at time FINTIM
FINXVL	Floating	8	16	8	Particle x-direction velocity along entire particle path
FINYVL	Floating	8	16	8	Particle y-direction velocity along entire particle path
FINZVL	Floating	8	16	8	Particle z-direction velocity along entire particle path
FINSPD	Floating	8	16	8	Particle speed along entire particle path
FINDIS	Floating	8	16	3	Distance along entire particle path
MODSTP	Integer	10	10	0	Cumulative MODFLOW time step number (Pollock, 1994, p. B–4)
IPCODE	Integer	10	10	0	Particle termination code (Pollock, 1994, p. B–4)
IDCODE	Integer	10	10	0	Particle discharge code (Pollock, 1994, p. B–4)
RESTIM	Floating	8	16	3	Release time (Pollock, 1994, p. B–4)

Table 7. Attributes associated with zones of transport GIS output from MODTOOLS

[n - width determined by MODTOOLS from model grid]

Attribute name	Item type	Input width	Output width	Number of decimals	Description
TIMSTP	Integer	10	10	0	Model time step from TIMESERS file output by MODPATH
PARTID	Binary	4	5	0	Particle-id from TIMESERS files output by MODPATH
STRTIM	Floating	8	16	3	Starting time of particle at time zero
STRROW	Integer	n	n	0	Starting row at time STRTIM
STRCOL	Integer	n	n	0	Starting column at time STRTIM
STRLAY	Integer	n	n	0	Starting model layer at time STRTIM
STRIBD	Integer	10	10	0	Starting model ibound value at time STRTIM
STRXGC	Floating	8	16	3	Starting global particle x-coordinate at time STRTIM
STRXLC	Floating	8	16	3	Starting local particle x-coordinate at time STRTIM
STRYGC	Floating	8	16	3	Starting global particle y-coordinate at time STRTIM
STRYLC	Floating	8	16	3	Starting local particle y-coordinate at time STRTIM
STRZGC	Floating	8	16	3	Starting global particle z-coordinate at time STRTIM
STRZLC	Floating	8	16	3	Starting local particle z-coordinate at time STRTIM
FINTIM	Floating	8	16	3	Final cumulative time of particle
FINROW	Integer	n	n	0	Final row at time FINTIM
FINCOL	Integer	n	n	0	Final column at time FINTIM
FINLAY	Integer	n	n	0	Final model layer at time FINTIM
FINIBD	Integer	10	10	0	Final model ibound value at time FINTIM
FINXGC	Floating	8	16	3	Final global particle x-coordinate at time FINTIM
FINXLC	Floating	8	16	3	Final local particle x-coordinate at time FINTIM
FINYGC	Floating	8	16	3	Final global particle y-coordinate at time FINTIM
FINYLC	Floating	8	16	3	Final local particle y-coordinate at time FINTIM
FINZGC	Floating	8	16	3	Final global particle z-coordinate at time FINTIM
FINZLC	Floating	8	16	3	Final local particle z-coordinate at time FINTIM
FINXVL	Floating	8	16	6	Particle x-direction velocity along entire particle path
FINYVL	Floating	8	16	6	Particle y-direction velocity along entire particle path
FINZVL	Floating	8	16	6	Particle z-direction velocity along entire particle path
FINSPD	Floating	8	16	6	Particle speed along entire particle path
FINDIS	Floating	8	16	3	Distance along entire particle path
MODSTP	Integer	10	10	0	MODFLOW time step number
IPCODE	Integer	10	10	0	Particle termination code (Pollock, 1994, p. B–4)
IDCODE	Integer	10	10	0	Particle discharge code (Pollock, 1994, p. B–4)
RESTIM	Floating	8	16	3	Release time (Pollock, 1994, p. B–4)

Table 8. Attributes associated with model-grid GIS output from MODTOOLS
[n, width determined by MODTOOLS from model grid]

Attribute name	Item type	Input width	Output width	Number of decimals	Description
xxxID	Binary	4	5	0	Id identifying the polygons output by MODTOOLS
ROW	Integer	n	n	0	Row in the model grid
COLUMN	Integer	n	n	0	Column in the model grid
LAYER	Integer	n	n	0	Layer in the model grid
IBOUND	Integer	10	10	0	Value of IBOUND array for this cell
TOPELEV	Floating	8	16	3	Top elevation of cell in global z-coordinate units
BOTELEV	Floating	8	16	3	Bottom elevation of cell in global z-coordinate units
THICK	Floating	8	16	3	Thickness of cell in global z-coordinate units

Output from MODFLOW

MODTOOLS creates three types of GIS output from MODFLOW data: contour, velocity-vector, and cell-value files. MODTOOLS omits cells from GIS output on the basis of several conditions. Cells that are inactive (cell IBOUND = 0) are automatically omitted. For cell values, cells that have a value equal to the user-specified value for dry cells (HDRY item in MAIN file) or for no-flow cells (HNOFLO item in MAIN file) are omitted. Also, the user can choose to output the cell values for cells in a specified layer, for cells with a specific IBOUND value, or for the uppermost active cells.

For contour and velocity-vector GIS output, MODTOOLS uses the "normalized" approach (Pollock, 1994, p. 4–12) for vertical profiles instead of a global system for mapview perspectives. MODTOOLS computes an average thickness for each model layer and constructs a rectangular cross section with layers of constant thickness. This approach is used for a contour GIS output only for vertical profile views, because the computer program CONTOUR developed by Harbaugh (1990) was designed only for a mapview perspective and to work with gridded data of MODFLOW. CONTOUR has been adapted to work for vertical profile views, but cells with constant thickness must be used considering the numerical problems caused by vertical discretization schemes. This same approach produced better plots for a velocity-vector GIS output in vertical profile views, because the varying thicknesses of the grid cells caused by vertical discretization schemes produced less desirable results.

Contour Data

MODTOOLS constructs contour GIS output from cell-by-cell terms recorded in the CONTOUR-DATA file identified in the NAME file. MODTOOLS incorporates a contouring package that is adapted directly from the program developed and described by Harbaugh (1990). MODTOOLS reads the cell-by-cell terms of MODFLOW and computes a set of lines connecting points of equal value. MODTOOLS reads formatting information recorded in the CONTOUR-CONTROL file identified in the NAME file to properly read the cell-by-cell terms.

MODTOOLS allows the user several options for orientation. MODTOOLS constructs only a contour GIS output if the user specifies a mapview orientation. MODTOOLS constructs a contour GIS output and a separate model-grid GIS output showing the cell geometry if the user specifies a vertical profile orientation along a specified row or column of the model grid or along a specified particle pathline read from the PATHLINE file. The two GIS outputs created for vertical profile orientations use the local coordinate system and the user can combine the digital images into one display or plot using the capabilities of the GIS. MODTOOLS records the value of the contour line in an attribute called CONTOUR in the contour GIS output.

Velocity-Vector Data

MODTOOLS constructs velocity-vector GIS output using a flow-vector routine that is adapted from MMSP (modular model statistical processor) developed for MODFLOW by Scott (1990, p. 62). MODTOOLS constructs velocity vectors (representing average interstitial velocity) using this routine and additional information from the cell geometry and porosity arrays used by MODPATH and from the simulated head and cell-by-cell flow terms output by the Basic and the Block Centered Flow Packages of MODFLOW. MODTOOLS reads the cell geometry and porosity data from the MAIN file identified in the NAME file. MODTOOLS reads the cell-by-cell terms output by the Block Centered Flow Package of MODFLOW and recorded in the BUDGET file identified in the NAME file. MODTOOLS also reads the head values output by the Basic Package of MODFLOW and recorded in the HEAD or HEAD(BINARY) file identified in the NAME file.

MODTOOLS computes the orthogonal components (x, y, and z) of flow in each active cell in a manner similar to that used by the flow-vector routine of MMSP (Scott, 1990, p. 62–64). However, MODTOOLS computes the velocity vector by dividing the volumetric flow components by the product of the cross-sectional area of saturated flow and the effective porosity of the cell. The length of the velocity vector is determined by multiplying the velocity component by a user-specified scaling value. MODTOOLS uses the user-specified viewing orientation to determine which two orthogonal components of the velocity to use when computing the direction of the line representing the velocity vector (x-y, x-z, or y-z).

MODTOOLS allows the length of velocity vectors to be scaled either arithmetically or logarithmically. When arithmetic scaling is selected, the length of each velocity vector is multiplied by a user-specified constant. When logarithmic scaling is selected, the length of each velocity vector is multiplied by a computed constant. The computed constant is the product of the absolute value of the user-specified constant and the minimum power-of-10 multiplier needed to increase the minimum nonzero vector length to a value greater than one (Scott, 1990, p. 64).

MODTOOLS allows the user several options in the viewing orientation. MODTOOLS constructs only a velocity-vector GIS output if the user specifies a mapview orientation. MODTOOLS constructs a velocity-vector GIS output and a separate model-grid GIS output showing the cell geometry for vertical profiles along a specified row or column of the model grid. The two GIS outputs created for vertical profile orientations use the local coordinate system and can be combined into one display or plot using

the capabilities of the GIS. MODTOOLS computes up to 12 attributes for each vector depending upon the orientation of the view (table 9).

Table 9. Attributes associated with velocity-vector GIS output from MODTOOLS
[n - width determined by MODTOOLS from model grid]

Attribute name	Item type	Input width	Output width	Number of decimals	Descriptions
ROWCOL	character	n	n	0	Combined row and column item
ROW	Integer	n	n	0	Row in the model grid
COLUMN	Integer	n	n	0	Column in the model grid
LAYER	Integer	n	n	0	Layer in the model grid
IBOUND	Integer	10	10	0	Value of IBOUND array for this cell
LAYER_	Floating	8	16	3	Value of cell-by-cell term
XVELOCITY	Floating	8	16	3	Value of velocity vector in the x-direction of the model grid
YVELOCITY	Floating	8	16	3	Value of velocity vector in the y-direction of the model grid
ZVELOCITY	Floating	8	16	3	Value of velocity vector in the z-direction of the model grid
XYSPEED	Floating	8	16	3	Value of flow speed in the x-y plane of the model grid
XZSPEED	Floating	8	16	3	Value of flow speed in the x-z plane of the model grid
YZSPEED	Floating	8	16	3	Value of flow speed in the y-z plane of the model grid

Cell-Value Data

MODTOOLS reads the cell-by-cell terms of MODFLOW and records a set of attributes associated with each cell to the GIS file(s) or appends the cell values to the set of attributes associated with each cell of a model-grid GIS output (see table 8 for cell attributes). The user may select the stress period and time step of the cell values. MODTOOLS constructs a model-grid GIS output showing the cell geometry in vertical profiles along a specified row or column of the model grid and along a specified particle pathline read from the PATHLINE file. The cell values of MODFLOW are appended to the cell attributes.

When the user has specified a mapview orientation, MODTOOLS reads the cell-by-cell terms output by the user-specified package of MODFLOW and records a set of attributes associated with each cell to a GIS file(s). The names and definitions of these attributes are shown in table 10. The names and the number of attributes are determined by the package of MODFLOW selected by the user and the type of mapview orientation. The user can choose to record cell-by-cell terms for all model Slayers to a GIS file. The value of each term is recorded in an item for each layer called LAYER_xx, where xx is the layer number.

Table 10. Attributes associated with cell-value GIS output from MODTOOLS (adapted from Pollock, 1994, p. A–7)

[n, width determined by MODTOOLS from model grid]

Attribute name	Item type	Input width	Output width	Number of decimals	Descriptions
xxxID	Binary	4	5	0	Id identifying the polygons output by MODTOOLS
SEQNUM	Integer	n	n	0	Sequential number assigned to cells
ROW	Integer	n	n	0	Row in the model grid
COLUMN	Integer	n	n	0	Column in the model grid
LAYER_xx	Integer	n	n	0	Layer in the model grid
IBOUND	Integer	10	10	0	Value of IBOUND array for this cell
LAYER	Floating	8	16	3	Value of cell-by-cell term
HEDTRM	Floating	8	16	3	Value of head from Basic Package
DDNTRM	Floating	8	16	3	Value of drawdown from Basic Package
FFFTRM	Floating	8	16	3	Value of flow through front face cell-by-cell term of Block Centered Flow Package
FLFTRM	Floating	8	16	3	Value of flow through lower face cell-by-cell term of Block Centered Flow Package
FRFTRM	Floating	8	16	3	Value of flow through right face cell-by-cell term of Block Centered Flow Package
STOTRM	Floating	8	16	3	Value of flow from storage term of the Block Centered Flow Package
RCHTRM	Floating	8	16	3	Value of cell-by-cell term of Recharge Package
WELTRM	Floating	8	16	3	Value of cell-by-cell term of Well Package
RIVTRM	Floating	8	16	3	Value of cell-by-cell term of River Package
STRTRM	Floating	8	16	3	Value of cell-by-cell term of Streamflow Routing Package
STRFLO	Floating	8	16	3	Value of cell-by-cell streamflow of Streamflow Routing Package
DRNTRM	Floating	8	16	3	Value of cell-by-cell term of Drain Package
GHBTRM	Floating	8	16	3	Value of cell-by-cell term of General Head Boundary Package
EVTTRM	Floating	8	16	3	Value of cell-by-cell term of Evapotranspiration Package
IBSTRM	Floating	8	16	3	Value of cell-by-cell term of Interbed Storage Package
ARRTRM	Floating	8	16	8	Value of miscellaneous gridded model data

This file structure matches the file structure used by MODFLOWARC (Orzol and McGrath, 1992). Also, an item called SEQNUM (a unique model-cell identifier in the row-column plane) has been added to the set of attributes so that the GIS output from MODTOOLS is compatible with the GIS output from the MODELGRID programs (Kernodle and Philip, 1988). The user can choose to record cell values for a specific layer to a GIS file. The value of each term is recorded in an item for the specific layer called LAYER_xx. The user can choose to record cell values for cells which have a specific IBOUND value to a GIS file (see discussion by Pollock, 1994, p. 3–7). The sum of the terms is recorded in an item called IBOUND. The user can choose to record cell values for the uppermost active cells to a GIS file. The value of each term is recorded in an item for each uppermost active cell called xxxTRM, where xxx is generally a string of three characters similar to the character string identifying the MODFLOW package in the MODPATH NAME file developed by Pollock (1994, p. A6 to A7). For example, the user may choose to record the cell-by-cell terms output by the Drain Package of MODFLOW in a GIS file for the uppermost active cells. The values of these terms would be recorded in an item called DRNTRM.

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APPENDIXES

APPENDIX A. OBTAINING AND INSTALLING MODTOOLS

The computer programs described in this report are designed to translate data from the USGS modular finite-difference ground-water flow model (commonly known as MODFLOW) and particle-tracking programs (commonly known as MODPATH) into GIS files. The programs, named MODTOOLS, are available for downloading over the Internet from a USGS software repository. The repository is accessible on the World Wide Web (WWW) from the USGS Water Resources Information Web page at URL **http://water.usgs.gov/**. The URL for the public repository is: **http://water.usgs.gov/software/**. The public anonymous FTP site is on the Water Resources Information server (water.usgs.gov or 130.11.50.175) in the /pub/software/ground_water/modtools directory. When this code is revised or updated in the future, new versions or releases will be made available for downloading from these same sites.

MODTOOLS should work on any computer that has ARC/INFO software and has the capability to use AML programs. It has been tested on a Data General AViiON Unix workstation. MODTOOLS conforms to the FORTRAN-77 programming standard and, therefore, can be compiled on virtually any computer with a FORTRAN-77 compiler.

Installation involves three major steps: (1) copying and restoring the MODTOOLS directories onto your computer system, (2) editing the MODTOOLS AML programs, and (3) compiling the MODTOOLS FORTRAN programs. There are many public-domain and standard UNIX software programs that have the ability to restore the compressed MODTOOLS directory system.

For the AML programs of MODTOOLS to work properly, the user must edit two pathnames in the AML program called MODTOOLS.AML. The first pathname is on a line identified by the keywords "&s aml_path" and is followed by the pathname to the directory containing the AML programs. The user must edit the pathname to the directory where the MODTOOLS AML programs are restored. The second pathname is on the next line in MODTOOLS.AML. The user must edit the pathname to the directory where the MODTOOLS FORTRAN programs are restored.

For the FORTRAN programs of MODTOOLS to work properly, the following two steps must be done: (1) compile the FORTRAN programs of MODTOOLS and (2) link these programs of MODTOOLS and, if needed, link computer system libraries to produce an executable program. A file called MAKEFILE is included in the directory containing the FORTRAN programs. The user is encouraged to use this file to compile and link the MODTOOLS FORTRAN programs (see the UNIX "**make**" command for more information).

APPENDIX B. FILES AND MENU RESPONSES FOR EXAMPLES

Example 1: Particle Pathlines

NAME File

The MODTOOLS NAME file listed below was used to produce GIS output of each of the four pathline analyses shown in figure 3. The user will need to rename the particle endpoint and pathline data files after each analysis. Four PATHLINE files are required for example 1. The user could omit all files, except the files identified by the keywords MAIN and PATHLINE. In this case, MODTOOLS uses the MODPATH NAME file of the pathline analysis from the transient flow problem developed by Pollock (1994, p. E–33) for problem 2, run 1.

```
main            10   demo-t.mdf
wel             11   demo-t.wel
riv             12   demo-t.riv
rch             13   demo-t.rch
budget          50   demo-t.bud
head(binary)    60   demo-t.hed
cbf             70   demo-t.cbf
endpoint        75   endpoint.t1
pathline        76   pathline.t1
```

Menu Responses

The following is a list of menu responses necessary to reproduce the pathline GIS output during an interactive session between the user and MODTOOLS for example 1. After creating the first pathline GIS output from the particle-tracking analysis at a time of 500 years, the user can use the batch file that MODTOOLS created to automatically produce the pathline GIS output for the remaining three simulation times of 501, 503, 510 years.

Because the particle coordinates and attributes computed by MODTOOLS were not translated into another coordinate system, the user answers using the "none" option to multiplier and origin menus. However, these menus would generally be used to translate particle coordinates from MODPATH coordinates to GIS coordinates.

```
Select a MODTOOLS option for creating a coverage or info file(s)
-----------------------------------------------------------------
<cr> = Quit
  p = Pathline output
  e = Endpoint output
  t = Times-series output
  z = Zones-of-transport output
  g = Model-grid output
  c = Contour output
  v = Velocity-vector output
  i = Cell-value output
  h = Help
```

```
   Enter option:
p
...Particle pathline coverage selected


Select an orientation for the MODTOOLS GIS output
-----------------------------------------------------------------
<cr> = Quit
   m = Mapview
   r = Vertical profile view along a row
   c = Vertical profile view along a column
   p = Vertical profile view along a user-specified particle path
   h = Help
   b = Back to MODTOOLS Options menu

   Select an orientation:
m
...Mapview coverage


X,Y coordinate conversion
 Select option to convert from model units to GIS length units.
  (Note: For vertical profile orientations, MODTOOLS requires
  coordinates in units of feet).
-----------------------------------------------------------------
<cr> = Quit
   0 = None
   1 = Feet to meters
   2 = Meters to feet
   User-specified multiplication factor
   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter option:
0


Z coordinate conversion
 Select option to convert from model units to GIS length units.
  (Note: For vertical profile orientations, MODTOOLS requires
  coordinates in units of feet).
-----------------------------------------------------------------
<cr> = Quit
   0 = None
   1 = Feet to meters
   2 = Meters to feet
   User-specified multiplication factor
   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter option:
0


counterclockwise rotation angle around MODFLOW origin
-----------------------------------------------------------------
<cr> = Quit
   0 = None
   User-specified rotation angle
   h = Help
   b = Back to MODTOOLS Orientation menu

  Enter counterclockwise rotation angle:
0
```

APPENDIX B. FILES AND MENU RESPONSES FOR EXAMPLES—CONTINUED

```
X-origin of MODFLOW grid
-------------------------------------------------------------------
<cr> = Quit
    0 = None
    User-specified X-origin coordinate
    h = Help
    b = Back to MODTOOLS Orientation menu

  Enter x-origin:
0

Y-origin of MODFLOW grid
-------------------------------------------------------------------
<cr> = Quit
    0 = None
    User-specified Y-origin coordinate
    h = Help
    b = Back to MODTOOLS Orientation menu

  Enter y-origin:
0
```

Batch File

The following listing is from the batch file, MODTOOLS.OUT, which contains a summary of the menu responses necessary to reproduce the pathline GIS output created during the above interactive session between the user and MODTOOLS for example 1.

```
            0 NO MODPATH TRACKING OPTION NEEDED
            1 PARTICLE PATHLINE COVERAGE
      1.00000 NO X-Y-DIRECTION MULTIPLIER
      1.00000 NO Z-DIRECTION MULTIPLIER
      0.00000 ANGLE COUNTERCLOCKWISE ROTATION UPPER LEFT CORNER
      0.00000 X ORIGIN OF UPPER LEFT CORNER
      0.00000 Y ORIGIN OF UPPER LEFT CORNER
      1.00000 NO VERTICAL EXAGGERATION
      1.00000 NO HORIZONTAL MAP SCALE
            0 MAPVIEW ORIENTATION
            0 UNUSED FOR MAPVIEW ORIENTATION
            0 NO 2-D CONTOUR ARRAY
      0.00000 NO CONTOUR INTERVAL
            0 NO EQUAL SECTORS
     999.90    HYDRAULIC HEAD ASSIGNED TO NO-FLOW CELLS
   0.10000E+31 HYDRAULIC HEAD ASSIGNED TO DRY CELLS
```

Example 2: Particle Endpoints

NAME File

The MODTOOLS NAME file listed below was used to produce the endpoint GIS output for the endpoint analysis shown in figure 4. MODTOOLS needs only two data files from the list to construct the endpoint GIS output. The user could omit all files, except the files identified by the keywords MAIN and ENDPOINT. In this case, MODTOOLS uses the MODPATH NAME file of the endpoint analysis from the transient flow problem for problem 2, run 3 developed by Pollock (1994, p. E–33).

```
main          10  demo-t.mdf
wel           11  demo-t.wel
riv           12  demo-t.riv
rch           13  demo-t.rch
budget        50  demo-t.bud
head(binary)  60  demo-t.hed
cbf           70  demo-t.cbf
endpoint      75  endpoint.t3
```

Menu Responses

The following is a list of menu responses necessary to reproduce the endpoint GIS output during an interactive session between the user and MODTOOLS for example 2. After creating an endpoint GIS output from a particle-tracking analysis, the user can use the batch file that MODTOOLS created to automatically produce another endpoint GIS output for a different arrangement of starting particle locations to test an alternative scenario.

```
Select a MODTOOLS option for creating a coverage or info file(s)
----------------------------------------------------------------------
<cr> = Quit
   p = Pathline output
   e = Endpoint output
   t = Times-series output
   z = Zones-of-transport output
   g = Model-grid output
   c = Contour output
   v = Velocity-vector output
   i = Cell-value output
   h = Help

   Enter option:
e
...Particle locations coverage selected


Select a Modtools Option for creating a point coverage of starting or final locations
----------------------------------------------------------------------
<cr> = Quit
   s = Mapview of starting locations (forward tracking)
   f = Mapview of final locations (forward tracking)
   e = Mapview of final locations (backward tracking)
   h = Help on tracking mode by MODPATH
   b = Back to MODTOOLS Options menu

   Enter tracking mode
s

X,Y coordinate conversion
 Select option to convert from model units to GIS length units.
  (Note: For vertical profile orientations, MODTOOLS requires
  coordinates in units of feet).
----------------------------------------------------------------------
<cr> = Quit
   0 = None
   1 = Feet to meters
   2 = Meters to feet
   User-specified multiplication factor
   h = Help
   b = Back to MODTOOLS Orientation menu
```

```
   Enter option:
0

Z coordinate conversion
 Select option to convert from model units to GIS length units.
  (Note: For vertical profile orientations, MODTOOLS requires
  coordinates in units of feet).

-----------------------------------------------------------------
<cr> = Quit
    0 = None
    1 = Feet to meters
    2 = Meters to feet
    User-specified multiplication factor
    h = Help
    b = Back to MODTOOLS Orientation menu

   Enter option:
0

counterclockwise rotation angle around MODFLOW origin
-----------------------------------------------------------------
<cr> = Quit
    0 = None
    User-specified rotation angle
    h = Help
    b = Back to MODTOOLS Orientation menu

  Enter counterclockwise rotation angle:
0

X-origin of MODFLOW grid
-----------------------------------------------------------------
<cr> = Quit
    0 = None
    User-specified X-origin coordinate
    h = Help
    b = Back to MODTOOLS Orientation menu

  Enter x-origin:
0

Y-origin of MODFLOW grid
-----------------------------------------------------------------
<cr> = Quit
    0 = None
    User-specified Y-origin coordinate
    h = Help
    b = Back to MODTOOLS Orientation menu

  Enter y-origin:
0
```

Batch File

The following listing is from the batch file, MODTOOLS.OUT, which contains a summary of the menu responses necessary to reproduce the endpoint GIS output created during the above interactive session between the user and MODTOOLS for example 2.

APPENDIX B. FILES AND MENU RESPONSES FOR EXAMPLES—CONTINUED

Example 3: Particle Time-Series

NAME File

The MODTOOLS NAME file listed below was used to produce particle GIS output for the time-series analysis shown in figure 5. MODTOOLS needs only two data files from the list to construct the time-series GIS output. The user could omit all files, except the files identified by the keywords MAIN and TIME-SERIES. In this case, MODTOOLS uses the MODPATH NAME file from the steady-state flow problem developed by Pollock (1994, p. E–6) for problem 1, run 4.

```
        1 FORWARD TRACKING FOR MODPATH
        2 STARTING PARTICLE COVERAGE (FORWARD TRACKING)
  1.00000 NO X-Y-DIRECTION MULTIPLIER
  1.00000 NO Z-DIRECTION MULTIPLIER
  0.00000 ANGLE COUNTERCLOCKWISE ROTATION UPPER LEFT CORNER
  0.00000 X ORIGIN OF UPPER LEFT CORNER
  0.00000 Y ORIGIN OF UPPER LEFT CORNER
  1.00000 NO VERTICAL EXAGGERATION
  1.00000 NO HORIZONTAL MAP SCALE
        0 MAPVIEW ORIENTATION
        0 UNUSED FOR MAPVIEW ORIENTATION
        0 NO 2-D CONTOUR ARRAY
  0.00000 NO CONTOUR INTERVAL
        0 NO EQUAL SECTORS
  999.90     HYDRAULIC HEAD ASSIGNED TO NO-FLOW CELLS
0.10000E+31 HYDRAULIC HEAD ASSIGNED TO DRY CELLS
```

```
main          10   demo-s.mdf
wel           11   demo-s.wel
riv           12   demo-s.riv
rch           13   demo-s.rch
budget        50   demo-s.bud
head(binary)  60   demo-s.hed
endpoint      75   endpoint.s4
time-series   77   timesers.s4
```

Menu Responses

The following is a list of menu responses necessary to reproduce the time-series GIS output during an interactive session between the user and MODTOOLS for example 3. After creating the time-series GIS output from the particle-tracking analysis, the user can use the batch file that MODTOOLS created to automatically produce another time-series GIS output for a different set of multiple release times of travel to test an alternative scenario.

```
Select a MODTOOLS option for creating a coverage or info file(s)
----------------------------------------------------------------------
<cr> = Quit
   p = Pathline output
   e = Endpoint output
   t = Times-series output
   z = Zones-of-transport output
   g = Model-grid output
   c = Contour output
   v = Velocity-vector output
   i = Cell-value output
   h = Help

   Enter option:
t
...Time series coverage selected

Select an orientation for the MODTOOLS GIS output
----------------------------------------------------------------------
<cr> = Quit
   m = Mapview
   r = Vertical profile view along a row
   c = Vertical profile view along a column
   p = Vertical profile view along a user-specified particle path
   h = Help
   b = Back to MODTOOLS Options menu


    Select an orientation:
r
...Row vertical profile coverage


X,Y coordinate conversion
 Select option to convert from model units to GIS length units.
  (Note: For vertical profile orientations, MODTOOLS requires
  coordinates in units of feet).
----------------------------------------------------------------------
<cr> = Quit
   0 = None
   1 = Feet to meters
   2 = Meters to feet
   User-specified multiplication factor
   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter option:
0


Z coordinate conversion
 Select option to convert from model units to GIS length units.
  (Note: For vertical profile orientations, MODTOOLS requires
  coordinates in units of feet).
----------------------------------------------------------------------
<cr> = Quit
   0 = None
   1 = Feet to meters
   2 = Meters to feet
   User-specified multiplication factor
   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter option:
0
```

```
Enter vertical exaggeration
---------------------------------------------------------------------
<cr> = Quit
   User-specified vertical exaggeration factor
   h = Help
   b = Back to MODTOOLS Orientation menu


Enter vertical exaggeration 1 foot = n feet:
10
...Vertical Scale 1 foot =         10.0000000000 feet


Enter horizontal mapscale
---------------------------------------------------------------------
<cr> = Quit
   User-specified horizontal mapscale
   h = Help
   b = Back to Vertical Exaggeration menu


Enter horizontal mapscale 1 foot = n feet:
1
...Horizontal Scale 1 foot =         1.0000000000 feet

Enter number of row to view
---------------------------------------------------------------------
<cr> = Quit
   any numeric = selection
   h = Help
   b = Back to MODTOOLS Orientation menu

  Enter selection:
14
```

Batch File

The following listing is from the batch file, MODTOOLS.OUT, which contains a summary of the menu responses necessary to reproduce the time-series GIS output created during the above interactive session between the user and MODTOOLS for example 3.

```
          0 NO MODPATH TRACKING OPTION NEEDED
          3 TIME_SERIES COVERAGE
    1.00000 NO X-Y-DIRECTION MULTIPLIER
    1.00000 NO Z-DIRECTION MULTIPLIER
    0.00000 NO ANGLE OF ROTATION FROM UPPER LEFT CORNER
    0.00000 NO X ORIGIN OF UPPER LEFT CORNER
    0.00000 NO Y ORIGIN OF UPPER LEFT CORNER
   10.00000 VERTICAL EXAGGERATION
    1.00000 HORIZONTAL MAP SCALE
          1 ROW TRAVERSE ORIENTATION
         14 ROW; TRAVERSE ALONG ROW DIRECTION
          0 NO 2-D CONTOUR ARRAY
    0.00000 NO CONTOUR INTERVAL
          0 NO EQUAL SECTORS
   999.90     HYDRAULIC HEAD ASSIGNED TO NO-FLOW CELLS
  0.10000E+31 HYDRAULIC HEAD ASSIGNED TO DRY CELLS
```

APPENDIX B. FILES AND MENU RESPONSES FOR EXAMPLES—CONTINUED

Example 4: Zones of Transport

NAME File

The MODTOOLS NAME file listed below was used to produce particle GIS output for the zones-of-transport analysis shown in figure 6. MODTOOLS needs only three data files from the list to construct the time-series GIS output. The user could omit all files, except the files identified by the keywords MAIN, TIME-SERIES, and ENDPOINT. In this case, MODTOOLS uses the MODPATH NAME file from the steady-state flow problem developed by Pollock (1994, p. E–6) for problem 1, run 2.

```
main           10  demo-s.mdf
wel            11  demo-s.wel
riv            12  demo-s.riv
rch            13  demo-s.rch
budget         50  demo-s.bud
head(binary)   60  demo-s.hed
endpoint       75  endpoint.s2
time-series    77  timesers.s2
```

Menu Responses

The following is a list of menu responses necessary to reproduce the zones-of-transport GIS output during an interactive session between the user and MODTOOLS for example 4. After creating the zones-of-transport GIS output from the particle-tracking analysis, the user can use the batch file that MODTOOLS created to automatically produce another time-series GIS output for a different arrangement of starting particle locations to test an alternative scenario.

```
Select a MODTOOLS option for creating a coverage or info file(s)
----------------------------------------------------------------
<cr> = Quit
   p = Pathline output
   e = Endpoint output
   t = Times-series output
   z = Zones-of-transport output
   g = Model-grid output
   c = Contour output
   v = Velocity-vector output
   i = Cell-value output
   h = Help

   Enter option:
z
...Zone_of_transport_areas coverage selected


Select an orientation for the MODTOOLS GIS output
-------------------------------------------------------------------
<cr> = Quit
   m = Mapview
   r = Vertical profile view along a row
   c = Vertical profile view along a column
   p = Vertical profile view along a user-specified particle path
   h = Help
   b = Back to MODTOOLS Options menu
```

```
   Select an orientation:
m
...Mapview coverage


X,Y coordinate conversion
 Select option to convert from model units to GIS length units.
  (Note: For vertical profile orientations, MODTOOLS requires
  coordinates in units of feet).
----------------------------------------------------------------------
<cr> = Quit
   0 = None
   1 = Feet to meters
   2 = Meters to feet
   User-specified multiplication factor
   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter option:
0


Z coordinate conversion
 Select option to convert from model units to GIS length units.
  (Note: For vertical profile orientations, MODTOOLS requires
  coordinates in units of feet).
----------------------------------------------------------------------
<cr> = Quit
   0 = None
   1 = Feet to meters
   2 = Meters to feet
   User-specified multiplication factor
   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter option:
0


counterclockwise rotation angle around MODFLOW origin
----------------------------------------------------------------------
<cr> = Quit
   0 = None
   User-specified rotation angle
   h = Help
   b = Back to MODTOOLS Orientation menu


   Enter counterclockwise rotation angle:
0


X-origin of MODFLOW grid
----------------------------------------------------------------------
<cr> = Quit
   0 = None
   User-specified X-origin coordinate
   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter x-origin:
0

Y-origin of MODFLOW grid
----------------------------------------------------------------------
<cr> = Quit
   0 = None
   User-specified Y-origin coordinate
   h = Help
   b = Back to MODTOOLS Orientation menu
```

```
   Enter y-origin:
0


Enter number of equal sectors used to delineate zones of transport
------------------------------------------------------------------
<cr> = Quit
   User-specified number of sectors
   h = Help
   b = Back to MODTOOLS Orientation menu

Enter number of equal sectors
33
```

Batch File

The following listing is from the batch file, MODTOOLS.OUT, which contains a summary of the menu responses necessary to reproduce the zone-of-transport GIS output created during the above interactive session between the user and MODTOOLS for example 4.

```
            0 NO MODPATH TRACKING OPTION NEEDED
            4 ZONES_OF_TRANSPORT_AREA COVERAGE
      1.00000 NO X-Y-DIRECTION MULTIPLIER
      1.00000 NO Z-DIRECTION MULTIPLIER
      0.00000 NO ANGLE OF ROTATION FROM UPPER LEFT CORNER
      0.00000 NO X ORIGIN OF UPPER LEFT CORNER
      0.00000 NO Y ORIGIN OF UPPER LEFT CORNER
      1.00000 NO VERTICAL EXAGGERATION
      1.00000 NO HORIZONTAL MAP SCALE
            0 MAPVIEW ORIENTATION
            0 UNUSED FOR MAPVIEW ORIENTATION
            0 NO 2-D CONTOUR ARRAY
      0.00000 NO CONTOUR INTERVAL
           33 NO EQUAL SECTORS
   999.90    HYDRAULIC HEAD ASSIGNED TO NO-FLOW CELLS
 0.10000E+31 HYDRAULIC HEAD ASSIGNED TO DRY CELLS
```

Example 5: Model Grid

NAME File

The MODTOOLS NAME file listed below was used to produce a model-grid GIS output shown in figure 7. MODTOOLS needs up to three data files from the list to construct the model-grid GIS output. The user could omit all files, except the files identified by the keywords MAIN, HEAD(BINARY), and PATHLINE. For a GIS output in map view, the user need only construct the MODTOOLS MAIN file. The file identified by the keywords HEAD(BINARY) would only be needed if the user specified a GIS output in the vertical profile view such as along a row of the model grid. MODTOOLS uses the values of the simulated head for the tops of the cells if layer 1 is a water-table layer. A previous particle-tracking pathline analysis is needed to construct a model-grid GIS output for a vertical profile orientation along a particle pathline. Only in this instance would the file identified by the keyword PATHLINE be included in the NAME file resulting in the additional construction of a pathline GIS output in vertical profile view along the specified particle.

```
main           10  demo-t.mdf
wel            11  demo-t.wel
riv            12  demo-t.riv
rch            13  demo-t.rch
budget         50  demo-t.bud
head(binary)   60  demo-t.hed
cbf            70  demo-t.cbf
endpoint       75  endpoint.t1
pathline       76  pathline.t1
```

Menu Responses

The following is a list of menu responses necessary to reproduce the model-grid GIS output during an interactive session between the user and MODTOOLS for example 5. After creating the model-grid GIS output from the particle-tracking analysis, the user can use the batch file that MODTOOLS created to automatically produce another pathline GIS output for a different particle to test an alternative scenario.

```
Select a MODTOOLS option for creating a coverage or info file(s)
----------------------------------------------------------------
<cr> = Quit
   p = Pathline output
   e = Endpoint output
   t = Times-series output
   z = Zones-of-transport output
   g = Model-grid output
   c = Contour output
   v = Velocity-vector output
   i = Cell-value output
   h = Help

   Enter option:
p
...Particle pathline coverage selected




Select an orientation for the MODTOOLS GIS output
----------------------------------------------------------------
<cr> = Quit
   m = Mapview
   r = Vertical profile view along a row
   c = Vertical profile view along a column
   p = Vertical profile view along a user-specified particle path
   h = Help
   b = Back to MODTOOLS Options menu

   Select an orientation:
p
...Particle vertical profile coverage


X,Y coordinate conversion
 Select option to convert from model units to GIS length units.
  (Note: For vertical profile orientations, MODTOOLS requires
  coordinates in units of feet).
----------------------------------------------------------------
<cr> = Quit
   0 = None
   1 = Feet to meters
   2 = Meters to feet
   User-specified multiplication factor
```

```
   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter option:
0


Z coordinate conversion
 Select option to convert from model units to GIS length units.
  (Note: For vertical profile orientations, MODTOOLS requires
  coordinates in units of feet).
-------------------------------------------------------------------
<cr> = Quit
   0 = None
   1 = Feet to meters
   2 = Meters to feet
   User-specified multiplication factor
   h = Help
   b = Back to MODTOOLS Orientation menu


   Enter option:
0


Enter vertical exaggeration
-------------------------------------------------------------------
<cr> = Quit
   User-specified vertical exaggeration factor
   h = Help
   b = Back to MODTOOLS Orientation menu


Enter vertical exaggeration 1 foot = n feet:
10
...Vertical Scale 1 foot =        10.0000000000 feet


Enter horizontal mapscale
-------------------------------------------------------------------
<cr> = Quit
   User-specified horizontal mapscale
   h = Help
   b = Back to Vertical Exaggeration menu


Enter horizontal mapscale 1 foot = n feet:
1
...Horizontal Scale 1 foot =        1.0000000000 feet
Enter number of particle-id to view
-------------------------------------------------------------------
<cr> = Quit
   any numeric = selection
   h = Help
   b = Back to MODTOOLS Orientation menu

  Enter selection:
1
```

Batch File

The following listing is from the batch file, MODTOOLS.OUT, which contains a summary of the menu responses necessary to reproduce the two GIS outputs (the particle pathline GIS output and the accompanying model-grid GIS output) during an interactive session between the user and MODTOOLS for example 5.

```
        0 NO MODPATH TRACKING OPTION NEEDED
        1 PARTICLE PATHLINE COVERAGE
  1.00000 NO X-Y-DIRECTION MULTIPLIER
  1.00000 NO Z-DIRECTION MULTIPLIER
  0.00000 NO ANGLE OF ROTATION FROM UPPER LEFT CORNER
  0.00000 NO X ORIGIN OF UPPER LEFT CORNER
  0.00000 NO Y ORIGIN OF UPPER LEFT CORNER
 10.00000 VERTICAL EXAGGERATION
  1.00000 HORIZONTAL MAP SCALE
        3 PARTICLE PATHLINE ORIENTATION
        1 PARTICLE; TRAVERSE ALONG PARTICLE DIRECTION
        0 NO 2-D CONTOUR ARRAY
  0.00000 NO CONTOUR INTERVAL
        0 NO EQUAL SECTORS
   999.90    HYDRAULIC HEAD ASSIGNED TO NO-FLOW CELLS
0.10000E+31 HYDRAULIC HEAD ASSIGNED TO DRY CELLS
```

Example 6: Contours of Input and Output Arrays

NAME File

The MODTOOLS NAME file listed below was used to produce a contour GIS output shown in figure 8. MODTOOLS needs three data files from the list to construct the contour GIS output. The user could omit all files, except the files identified by the keywords MAIN, CONTOUR-DATA, and CONTOUR-CONTROL. For a GIS output in map view, MODTOOLS only constructs one GIS output which consists of a set of lines connecting points of equal value. For a GIS output in vertical profile view, MODTOOLS also constructs a model-grid GIS output.

```
main            10  demo-s.mdf
wel             11  demo-s.wel
riv             12  demo-s.riv
rch             13  demo-s.rch
budget          50  demo-s.bud
head(binary)    60  demo-s.hed
contour-data    61  demo-s.hed
contour-control 62  demo-s.ctl
endpoint        75  endpoint.s2
time-series     77  timesers.s2
```

Menu Responses

The following is a list of menu responses necessary to reproduce the contour GIS output during an interactive session between the user and MODTOOLS for example 6. After creating the contour GIS output, the user can use the batch file that MODTOOLS created to automatically produce another contour GIS output for a different set of input or output arrays to test alternative scenarios.

```
Select a MODTOOLS option for creating a coverage or info file(s)
```

APPENDIX B. FILES AND MENU RESPONSES FOR EXAMPLES—CONTINUED

```
----------------------------------------------------------------------
<cr> = Quit
   p = Pathline output
   e = Endpoint output
   t = Times-series output
   z = Zones-of-transport output
   g = Model-grid output
   c = Contour output
   v = Velocity-vector output
   i = Cell-value output
   h = Help

   Enter option:
c
...Contour coverage selected

Select an orientation for the MODTOOLS GIS output
----------------------------------------------------------------------
<cr> = Quit
   l = Mapview of a user-specified model layer
   i = Mapview of a user-specified model ibound value
   u = Mapview of uppermost active cells
   r = Vertical profile view along a row
   c = Vertical profile view along a column
   h = Help
   b = Back to MODTOOLS Options menu

   Select an orientation:
l
...Model layer orientation

X,Y coordinate conversion
 Select option to convert from model units to GIS length units.
  (Note: For vertical profile orientations, MODTOOLS requires
  coordinates in units of feet).
----------------------------------------------------------------------
<cr> = Quit
   0 = None
   1 = Feet to meters
   2 = Meters to feet
   User-specified multiplication factor
   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter option:
0


Z coordinate conversion
 Select option to convert from model units to GIS length units.
  (Note: For vertical profile orientations, MODTOOLS requires
  coordinates in units of feet).
----------------------------------------------------------------------
<cr> = Quit
   0 = None
   1 = Feet to meters
   2 = Meters to feet
   User-specified multiplication factor
   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter option:
0
```

```
counterclockwise rotation angle around MODFLOW origin
----------------------------------------------------------------------
<cr> = Quit
   0 = None
   User-specified rotation angle
   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter counterclockwise rotation angle:
0


X-origin of MODFLOW grid
----------------------------------------------------------------------
<cr> = Quit
   0 = None
   User-specified X-origin coordinate
   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter x-origin:
0

Y-origin of MODFLOW grid
----------------------------------------------------------------------
<cr> = Quit
   0 = None
   User-specified Y-origin coordinate

   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter y-origin:
0

Enter number of model layer to view
----------------------------------------------------------------------
<cr> = Quit
   User-specified selection
   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter selection:
4
...Mapview using layer          4

Enter dimension of the gridded model data
----------------------------------------------------------------------
<cr> = Quit
   2 = two-dimensional array
   3 = three-dimensional array
   b = Back to MODTOOLS Orientation menu
   h = Help
Enter dimension of gridded data:
2
...2-D Contour Array


Enter contour interval
----------------------------------------------------------------------
<cr> = Quit
   User-specified contour interval
   b = Back to MODTOOLS Orientation menu
   h = Help


Enter contour interval:
2
```
...Contour interval =   2.0000000000

APPENDIX B. FILES AND MENU RESPONSES FOR EXAMPLES—CONTINUED

Batch File

The following listing is from the batch file, MODTOOLS.OUT, which contains a summary of the menu responses necessary to reproduce the cell-value GIS output created during the above interactive session between the user and MODTOOLS for example 6.

```
        0 NO MODPATH TRACKING OPTION NEEDED
        7 CONTOUR GIS OUTPUT
  1.00000 NO X-Y COORDINATE CONVERSION FACTOR
  1.00000 NO Z COORDINATE CONVERSION FACTOR
  0.00000 ANGLE COUNTERCLOCKWISE ROTATION AROUND MODFLOW ORIGIN
  0.00000 X ORIGIN OF MODFLOW GRID
  0.00000 Y ORIGIN OF MODFLOW GRID
  1.00000 NO VERTICAL EXAGGERATION
  1.00000 NO HORIZONTAL MAPSCALE
        4 MODEL LAYER MAPVIEW ORIENTATION
        4 LAYER
        2 2-D DATA ARRAY
  2.00000 CONTOUR INTERVAL
        0 NO SECTORS FOR DELINEATING ZONES OF TRANSPORT
   999.90    HYDRAULIC HEAD ASSIGNED TO NOFLOW CELLS
0.10000E+31 HYDRAULIC HEAD ASSIGNED TO DRY CELLS
```

Example 7: Velocity Vectors

NAME File

The MODTOOLS NAME file listed below was used to produce a velocity-vector GIS output shown in figure 9. MODTOOLS needs up to four data files from the list to construct the velocity-vector GIS output. The user could omit all files, except the files identified by the keywords MAIN, BUDGET, and HEAD or HEAD(BINARY). The HEAD-CONTROL file would only be needed if the user specified that a formatted head file would be the source of head data using the keyword HEAD in the NAME file. MODTOOLS uses information on the format of the file in the HEAD-CONTROL file to read the simulated heads in the HEAD file. MODTOOLS needs the values of the simulated head to compute a saturated thickness for each cell. For a GIS output in vertical profile view, MODTOOLS also constructs a model-grid GIS output.

```
main           10   demo-s.mdf
wel            11   demo-s.wel
riv            12   demo-s.riv
rch            13   demo-s.rch
budget         50   demo-s.bud
head(binary)   70   demo-s.hed
endpoint       75   endpoint.s1
```

Menu Responses

The following is a list of menu responses necessary to reproduce the velocity-vector GIS output during an interactive session between the user and MODTOOLS for example 7. After creating the

velocity-vector GIS output, the user can use the batch file that MODTOOLS created to automatically produce another velocity-vector GIS output for a different ground-water simulation.

```
Select a MODTOOLS option for creating a coverage or info file(s)
-----------------------------------------------------------------
<cr> = Quit
   p = Pathline output
   e = Endpoint output
   t = Times-series output
   z = Zones-of-transport output
   g = Model-grid output
   c = Contour output
   v = Velocity-vector output
   i = Cell-value output
   h = Help

   Enter option:
v
...MODFLOW flow direction coverage selected


Select an orientation for the MODTOOLS GIS output
-----------------------------------------------------------------
<cr> = Quit
   m = Mapview
   r = Vertical profile view along a row
   c = Vertical profile view along a column
   p = Vertical profile view along a user-specified particle path
   h = Help
   b = Back to MODTOOLS Options menu

   Select an orientation:
l
...Model layer orientation


X,Y coordinate conversion
 Select option to convert from model units to GIS length units.
  (Note: For vertical profile orientations, MODTOOLS requires
  coordinates in units of feet).
-----------------------------------------------------------------
<cr> = Quit
   0 = None
   1 = Feet to meters
   2 = Meters to feet
   User-specified multiplication factor
   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter option:
0


Z coordinate conversion
 Select option to convert from model units to GIS length units.
  (Note: For vertical profile orientations, MODTOOLS requires
  coordinates in units of feet).
-----------------------------------------------------------------
<cr> = Quit
   0 = None
   1 = Feet to meters
   2 = Meters to feet
   User-specified multiplication factor
   h = Help
   b = Back to MODTOOLS Orientation menu
```

```
    Enter option:
0


counterclockwise rotation angle around MODFLOW origin
-----------------------------------------------------------------------
<cr> = Quit
    0 = None
    User-specified rotation angle
    h = Help
    b = Back to MODTOOLS Orientation menu

   Enter counterclockwise rotation angle:
0

X-origin of MODFLOW grid
-----------------------------------------------------------------------
<cr> = Quit
    0 = None
    User-specified X-origin coordinate
    h = Help
    b = Back to MODTOOLS Orientation menu

   Enter x-origin:
0

Y-origin of MODFLOW grid
-----------------------------------------------------------------------
<cr> = Quit
    0 = None
    User-specified Y-origin coordinate
    h = Help
    b = Back to MODTOOLS Orientation menu

   Enter y-origin:
0

Enter number of model layer to view
-----------------------------------------------------------------------
<cr> = Quit
    User-specified selection
    h = Help
    b = Back to MODTOOLS Orientation menu

   Enter selection:
4
...Mapview using layer          4


Enter scaling factor for length of velocity vector
-----------------------------------------------------------------------
<cr> = Quit
    n > 0 - arithmetic scaling
    n = 0 - no scaling
    n < 0 - logarithmic scaling
    h = Help
    b = Back to MODTOOLS Orientation menu

Enter scaling factor:
-25
```

APPENDIX B. FILES AND MENU RESPONSES FOR EXAMPLES—CONTINUED

Batch File

The following listing is from the batch file, MODTOOLS.OUT, which contains a summary of the menu responses necessary to reproduce the velocity-vector GIS output created during the above interactive session between the user and MODTOOLS for example 7.

```
        0 NO MODPATH TRACKING OPTION NEEDED
        8 VELOCITY VECTORS GIS OUTPUT
  1.00000 NO X-Y-DIRECTION MULTIPLIER
  1.00000 NO Z-DIRECTION MULTIPLIER
  0.00000 ANGLE COUNTERCLOCKWISE ROTATION UPPER LEFT CORNER
  0.00000 X ORIGIN OF UPPER LEFT CORNER
  0.00000 Y ORIGIN OF UPPER LEFT CORNER
  1.00000 NO VERTICAL EXAGGERATION
  1.00000 NO HORIZONTAL MAP SCALE
        4 MODEL LAYER MAPVIEW ORIENTATION
        4 SINGLE MODEL LAYER MAPVIEW
        0 NO 2-D CONTOUR ARRAY
 -25.00000 LOGARITHMIC SCALING
        0 NO EQUAL SECTORS
   999.90    HYDRAULIC HEAD ASSIGNED TO NO-FLOW CELLS
 0.10000E+31 HYDRAULIC HEAD ASSIGNED TO DRY CELLS
```

Example 8: Cell Values

NAME File

The NAME file listed below was used to produce the cell-value GIS output shown in figure 10. MODTOOLS needs up to four data files from the list to construct the cell-value GIS output. The user could omit all files, except the files identified by the keywords MAIN, BUDGET, HEAD or AHEAD(BINARY), and PATHLINE. For a GIS output in map view, the user need only construct the MODPATH MAIN file and a MODTOOLS NAME file. The file identified by the keywords HEAD or HEAD(BINARY) would only be needed if the user specified a GIS output in the vertical profile view such as along a row of the model grid. MODTOOLS uses the values of the simulated head for the tops of the cells if layer 1 is a water-table layer. The one file identified by the keywords BUDGET or HEAD or HEAD(BINARY) would only be needed if the user specified this file as the source of the cell-by-cell terms. A particle-tracking analysis need only be done in order for MODTOOLS to construct a cell-value GIS output along a particle pathline. Only in this instance would the file identified by the keyword PATH-LINE be included in the NAME file resulting in the additional construction of a pathline GIS output in vertical profile view along the specified particle.

```
main           10   demo-t.mdf
wel            11   demo-t.wel
riv            12   demo-t.riv
rch            13   demo-t.rch
budget         50   demo-t.bud
head(binary)   60   demo-t.hed
cbf            70   demo-t.cbf
endpoint       75   endpoint.t1
pathline       76   pathline.t1
```

Menu Responses

The following is a list of menu responses necessary to reproduce the cell-value GIS output during an interactive session between the user and MODTOOLS for example 8. After creating the cell-value GIS output, the user can use the batch file that MODTOOLS created to automatically produce another cell-value GIS output for a different set of terms to test an alternative scenario.

```
Select a MODTOOLS option for creating a coverage or info file(s)
-----------------------------------------------------------------
<cr> = Quit
   p = Pathline output
   e = Endpoint output
   t = Times-series output
   z = Zones-of-transport output
   g = Model-grid output
   c = Contour output
   v = Velocity-vector output
   i = Cell-value output
   h = Help

   Enter option:
i
...Cell-by-cell Info file selected


Select the cell-by-cell terms from MODFLOW
-----------------------------------------------------------------
<cr> = Quit
 hed = Head terms from Basic Package
 ddn = Drawdown terms from Basic Package
 bcf = Flow terms through cell faces from Block Centered Flow Package
 sto = Storage terms from Block Centered Flow Package
 riv = Flow terms from River Package
 rch = Flow terms from Recharge Package
 wel = Flow terms from Well Package
 drn = Flow terms from Drain Package
 ghb = Flow terms from General Head Boundary Package
 evt = Flow terms from Evapotranspiration Package
 str = Flow terms from Streamflow-Routing Package
 flo = Streamflow terms from Streamflow-Routing Package [flow]
 ibs = Storage terms from Interbed-Storage Package
 arr = Data array gridded like MODFLOW arrays
   h = Help
   b = Return to MODTOOLS Options menu

   Enter cell-by-cell term selection:
hed
...Cell-by-cell head terms from Basic Package




Select an orientation for the MODTOOLS GIS output
-----------------------------------------------------------------
<cr> = Quit
   m = Mapview, characteristics for all layers will be generated
   l = Mapview of a user-specified model layer
   i = Mapview of a user-specified model ibound value
   u = Mapview of uppermost active cells
   r = Vertical profile view along a row
   c = Vertical profile view along a column
   p = Vertical profile view along a user-specified particle path
   h = Help
   b = To return to MODTOOLS Options menu
```

```
   Select an orientation:
r
...Row vertical profile coverage


X,Y coordinate conversion
 Select option to convert from model units to GIS length units.
  (Note: For vertical profile orientations, MODTOOLS requires
  coordinates in units of feet).
----------------------------------------------------------------------
<cr> = Quit
   0 = None
   1 = Feet to meters
   2 = Meters to feet
   User-specified multiplication factor
   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter option:
0


Z coordinate conversion
 Select option to convert from model units to GIS length units.
  (Note: For vertical profile orientations, MODTOOLS requires
  coordinates in units of feet).
----------------------------------------------------------------------
<cr> = Quit
   0 = None
   1 = Feet to meters
   2 = Meters to feet
   User-specified multiplication factor
   h = Help
   b = Back to MODTOOLS Orientation menu

   Enter option:
0

Enter vertical exaggeration
----------------------------------------------------------------------
<cr> = Quit
   User-specified vertical exaggeration factor
   h = Help
   b = Back to MODTOOLS Orientation menu


Enter vertical exaggeration 1 foot = n feet:
10
...Vertical Scale 1 foot =       10.0000000000 feet


Enter horizontal mapscale
----------------------------------------------------------------------
<cr> = Quit
   User-specified horizontal mapscale
   h = Help
   b = Back to Vertical Exaggeration menu


Enter horizontal mapscale 1 foot = n feet:
1
...Horizontal Scale 1 foot =        1.0000000000 feet

Enter number of row to view
----------------------------------------------------------------------
<cr> = Quit
   any numeric = selection
   h = Help
   b = Back to MODTOOLS Orientation menu
```

```
   Enter selection:
14
...Row vertical profile using row         14


Enter MODFLOW stress period number for the cell-by-cell terms
----------------------------------------------------------------
<cr> = Quit
   User-specified stress period
   h = Help
   b = Back to MODTOOLS Orientation menu


Enter stress period number:
3
...Stress period =            3


Enter MODFLOW time step number for cell-by-cell terms
----------------------------------------------------------------
<cr> = Quit
   User-specified time step
   h = Help
   b = Back to MODTOOLS Orientation menu

Enter time step number:
1
```

Batch File

The following listing is from the batch file, MODTOOLS.OUT, which contains a summary of the
menu responses necessary to reproduce the cell-value GIS output created during the above interactive
session between the user and MODTOOLS for example 8.

```
            1 CELL-BY-CELL HEAD TERMS FROM BAS PACKAGE
            6 CELL_BY_CELL FLOW INFO FILE
      1.00000 NO X-Y-DIRECTION MULTIPLIER
      1.00000 NO Z-DIRECTION MULTIPLIER
      0.00000 NO ANGLE OF ROTATION FROM UPPER LEFT CORNER
      0.00000 NO X ORIGIN OF UPPER LEFT CORNER
      0.00000 NO Y ORIGIN OF UPPER LEFT CORNER
     10.00000 VERTICAL EXAGGERATION
      1.00000 HORIZONTAL MAP SCALE
            1 ROW TRAVERSE ORIENTATION
           14 ROW; TRAVERSE ALONG ROW DIRECTION
            0 NO 2-D CONTOUR ARRAY
            3 MODFLOW STRESS PERIOD
            1 MODFLOW TIME STEP
     999.90     HYDRAULIC HEAD ASSIGNED TO NO-FLOW CELLS
   0.10000E+31 HYDRAULIC HEAD ASSIGNED TO DRY CELLS
```

APPENDIX C. DOCUMENTATION OF THE METHOD USED TO CONSTRUCT ZONES OF TRANSPORT

MODTOOLS uses an algorithm that delineates an approximation of the zones of transport for a pumped well from particle data generated using the time-series option of MODPATH (Pollock, 1994) as particles are backward tracked from the cell(s) containing the pumped well. In the following discussions of the delineation algorithm, the starting particle positions are assigned independently of MODPATH and are input by file to MODPATH rather than using the internal routine in MODPATH. To achieve a better initial configuration of particles for example 4 (zones of transport), the starting particle positions were arranged on the surface of a vertical cylinder, the axis of which passes through the center of the model-grid cell containing the well. The length and diameter of the cylinder are equal to the thickness and width of the cell. Particles are placed around the perimeter of the cylinder in horizontal planes that are equally spaced along the cylinder's vertical length. To achieve a better distribution, each successive horizontal plane of particles is rotated clockwise about the vertical axis of the cylinder by $\dfrac{360}{n\,(m-1)}$ degrees, where n is the number of particles in the plane, and m is the number of planes. The number of particles and the number of planes are specified by the user. This method of specifying starting particle positions is referred to as the vertical-cylindrical positioning method.

The starting positions of particles used to determine the zone of transport define the surface of a volume, a cylinder in this case. This cylinder deforms as the particles representing its surface move backward through the ground-water flow system. Particles from adjacent planes may travel with velocities that vary widely, distorting the surface of the cylinder into a complex three-dimensional form, which is difficult to project on to a reference plane for the delineation of the zone of transport. The reference plane is generally a horizontal plane representing the top of the saturated part of the ground-water system. Because of this complexity, a simple method of delineating polygons, which describe the approximate zones of transport was devised for use in MODTOOLS.

The delineating algorithm used in MODTOOLS approximates the zone of transport for a time step by projecting the particles onto the reference plane and then determining the maximum extent of travel since the last time step within each equal pie-shaped area (or sector) of a circle centered on the originating cell. The approximate positions of the maximum extent for each sector are then joined to form a polygon representing the zone of transport for that time step.

Figure C1 shows an example of this method for a single time step using particles originating from a single horizontal plane of particles created using the vertical-cylindrical positioning method. The starting particles, located in the cell containing the well, move to new positions, recorded by MODPATH in the TIMESERS file, at the end of time step one (fig. C1a). MODTOOLS also incorporates ending particle positions, recorded by MODPATH in the ENDPOINT files. This ensures particle positions intercepting a model boundary, such as the water table, are included in the delineation of the zones of transport. The area is then divided into a user-specified number of equal pie-shaped sectors centered on the originating cell (fig. C1b). The algorithm starts by searching each sector for all particle positions associated with the first time step (from among all of the particles started using the vertical-cylindrical

## APPENDIX C. DOCUMENTATION OF THE METHOD USED TO CONSTRUCT ZONES OF TRANSPORT—CONTINUED

positioning method). The algorithm identifies the particle in each sector that has traveled farthest from the center of the originating cell (fig. C1c). This distance, r_1, is then used to locate a new point out from the center along the bisector, B, of the sector (fig. C1d). This new point (labeled v_1 in fig. C1d) becomes one of the vertices that, when connected to adjacent vertices calculated for the other sectors, defines a polygon representing the approximate zone of transport for the time step (fig. C1e). The polygon can be shaded using the plotting capabilities of the GIS (fig. C1f). The process is identical for subsequent time steps except that for each sector the maximum distance of a particle from the originating cell is selected among the current as well as all previous times steps to determine the vertex for the zone of transport polygon in that sector. This means the delineating algorithm does not select particles that have moved closer to the center of the originating cell. For an example, the particles were not selected that have moved towards the center of the originating cell and are within the polygon delineated for the starting positions (fig. C1a).

The example described above and presented in figure C1 shows only a single plane of particles started using the vertical-cylindrical positioning method. It must be emphasized, however, that to identify th17e particle that has traveled farthest from the center of the originating cell, the delineating algorithm searches all particles in the sector for a given time step, regardless of what horizontal plane the particles originated from.

MODTOOLS constructs two types of GIS output for zones of transport. The first type of output consists of the vertices of the polygons and the location, time, and velocity attributes associated with these vertices as derived from the characteristics of the particles farthest from the originating cell. The second type consists of the polygons that represent the approximate zones of transport for each time step.

The error in delineating zones of transport using this method is related to the initial arrangement (density) of particles relative to the model-grid cell spacing, the number of particles used in the analysis, the size and complexity of the polygon defining the true zone of transport, and the number of sectors (vertices) used to approximate the zone of transport. The relation of the error to the number of sectors and the size of the polygon defining the true zone of transport is illustrated in figure C2. Note that if no particles are located within a sector for a particular time step, the position of particles from the previous time step is used to locate the vertex of the zone of transport polygon for that sector. The presence of this situation is indicated by triangular gaps in the zone of transport polygon (see fig. 6). Using either more particles, fewer sectors, or more time steps can help minimize the problem. (Adding more particles should be tried first).

Increasing the number of starting particles reduces the possibility of producing triangular gaps and may also increase the definition of the boundaries of the zones of transport. Decreasing the length of individual time steps may result in zones-of-transport polygons that more closely approximate the true zones of transport. For particles with pathlines that move out of a sector,
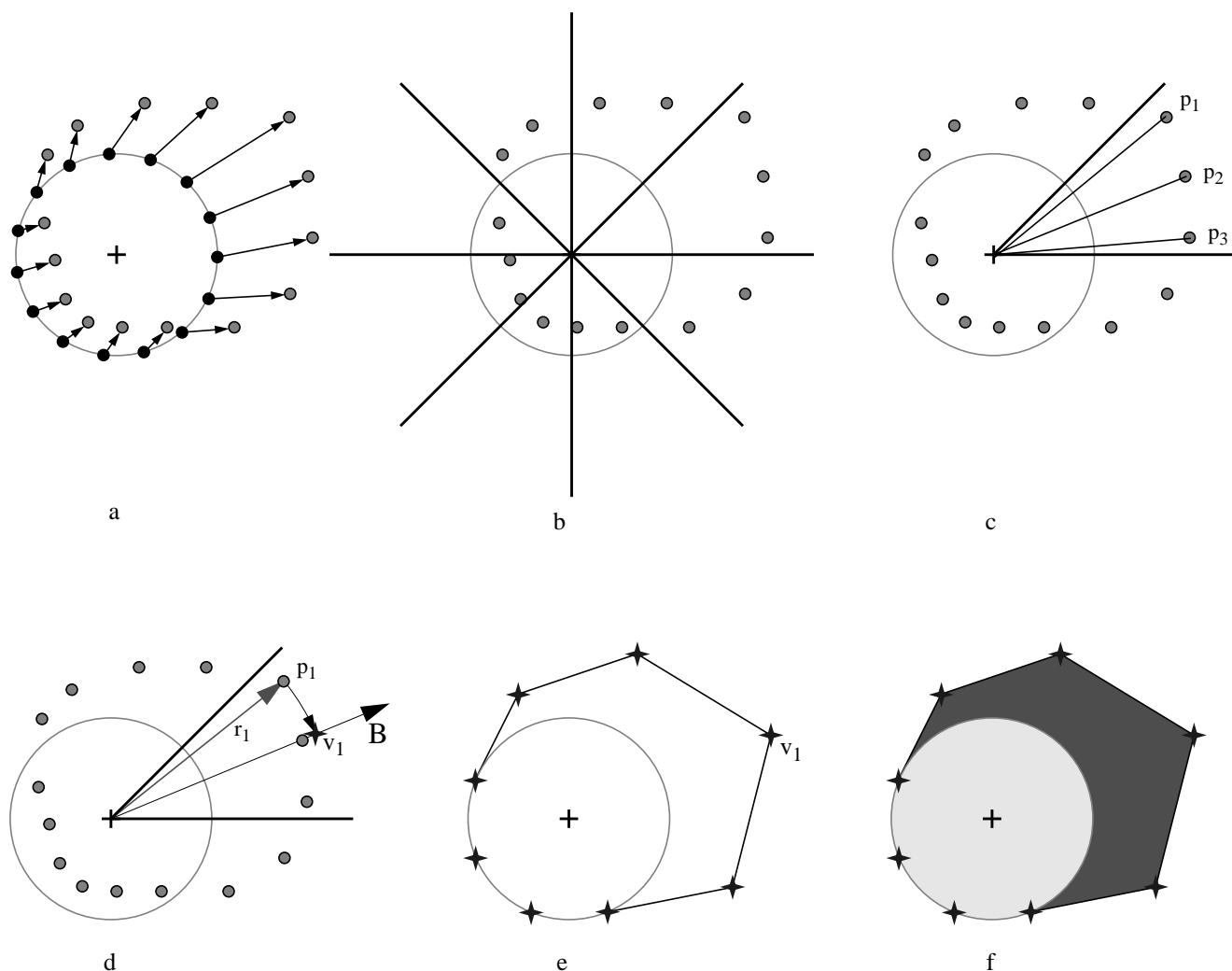
EXPLANATION

+ Center of cell containing pumped well
● Starting particle positions (shown only in fig. a and represented by circle in figs. b-f)
○ Particle positions at end of time step 1
✦ Position of vertex for zone of transport polygon

Figure C1. Example of steps used to construct polygons representing the approximate zones of transport for a cell containing a pumped well (seen in map view):   (a) The starting particle positions (as arranged using the vertical-cylindrical positioning method) and the particle positions at the end of a time step; (b) Division of area into a user-specified number of equal sectors; (c) The identification of the particle position (p_1) as farthest from the center of the originating cell among all particle positions within the sector (p_1 - p_3); (d) The creation of a vertex (v_1) along the bisector (B) of the sector at a distance equal to the farthest particle position (r_1); (e) Steps c-f have been repeated for each sector and the adjacent vertices for each sector joined to form a polygon representing the approximate zone of transport; (f) The polygon for the zone of transport shaded using the GIS. This process is repeated for each successive time step. Note that the example uses only a single horizontal plane or starting particles. Typically, multiple planes of particles are started. The same steps are used to construct the zone of transport but the search for the most distant particle by sector includes all particles in a sector regardless of which horizontal plane they were started in.
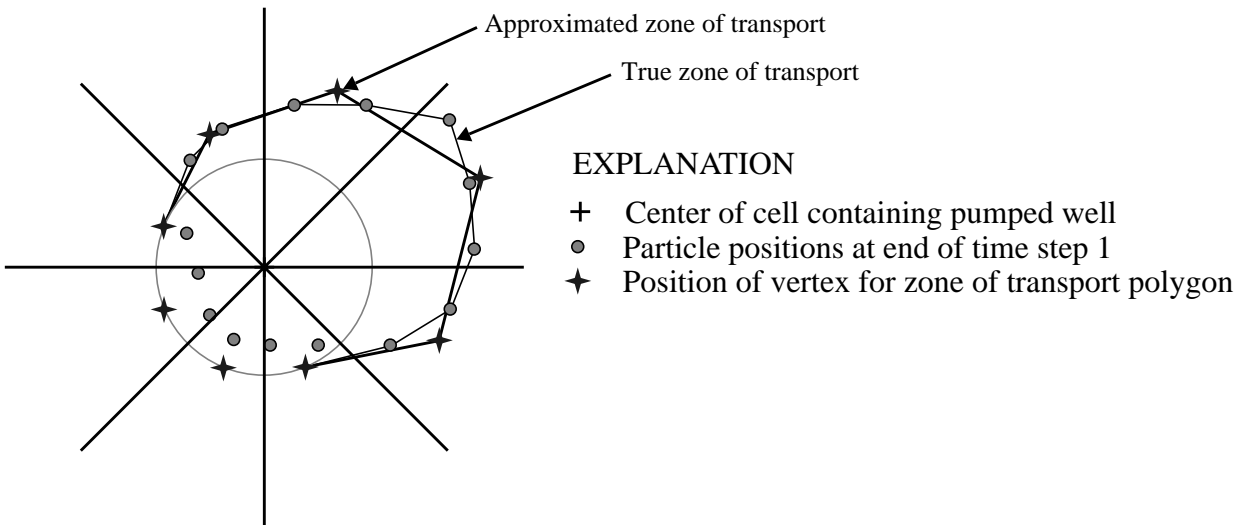
Figure C2. Approximated zone of transport delineated using the bisector method and the true zone of transport delineated by connecting particle positions.

shorter time steps may increase the probability that a particle will be present within the sector during a time step which can then be used to create a vertex for the approximated zone of transport. Longer time steps may be of sufficient duration that a particle moves out of the sector and is not used to create the vertex for that time step. The selection of an optimum number of sectors, number and arrangement of starting particles, and length of time steps will vary for each well and is influenced by the geometry and hydraulic characteristics of the ground-water flow system.

In the situation where much of the water discharging to a cell containing a well enters the cell through the top and bottom faces, placing particles on the top and bottom faces of the cell can produce a more accurate vertical representation of the zone of transport. To visualize a zone of transport in such situations, the user has the option of delineating the zone in a vertical profile view.