Processing Modflow

A Simulation System for Modeling Groundwater Flow and Pollution

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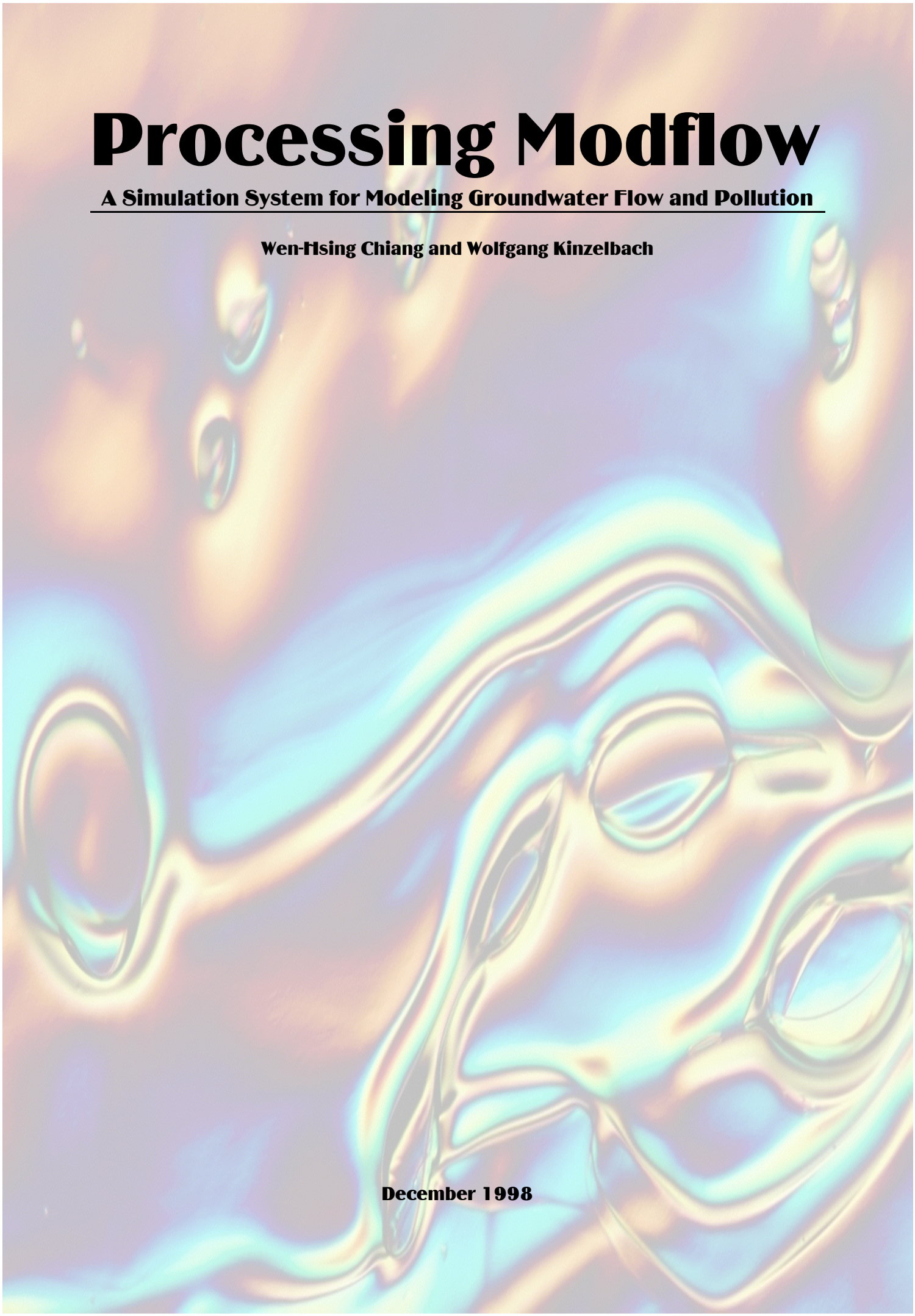

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Preface

Welcome to *Processing Modflow: A Simulation System for Modeling Groundwater Flow and Pollution*. Processing Modflow was originally developed for a remediation project of a disposal site in the coastal region of Northern Germany. At the beginning of the work, the code was designed as a pre- and postprocessor for the groundwater flow model MODFLOW. Several years ago, we began to prepare a Windows-version of Processing Modflow with the goal of bringing various codes together in a complete simulation system. The size of the program code grew, as we began to prepare the Windows-based advective transport model PMPATH and add options and features for supporting the solute transport models MT3D, MT3DMS and MOC3D and the inverse models PEST and UCODE.

As in the earlier versions of Processing Modflow, our goal is to provide an integrated groundwater modeling system with the hope that the very user-friendly implementation will lower the threshold which inhibits the widespread use of computer based groundwater models. To facilitate the use of Processing Modflow, more than 60 documented ready-to-run models are included in this software. Some of these models deal with theoretical background, some of them are of practical values.

The present text can be divided into three parts. The first two chapters introduce PMWIN with an example. Chapters 3 through 5 are a detalied description of the building blocks. Chapter 3 describes the use of Processing Modflow; chapter 4 describes the advection model PMPATH and chapter 5 introduces the modeling tools provided by Processing Modflow. The third part, Chapter 6, provides two tutorials and documents the examples.

Beside this text, we have gathered about 3,000 pages of documents related to the supported models. It is virtually not possible to provide all the documents in a printed form. So we decided to present these documents in an electronic format. The advantage of the electronic documents is considerable: with a single CD-ROM, you always have all necessary documents with you and we save resources by saving valuable papers and trees.

Many many people contributed to this modeling system. The authors wish to express heartfelt thanks to researchers and scientists, who have developed and coded the simulation programs MODFLOW, MOC3D, MT3D, MT3DMS, PEST and UCODE. Without their contributions, Processing Modflow would never have its present form. Many thanks are also due to authors of numerous add-on packages to MODFLOW.

We wish to thank many of our friends and colleagues for their contribution in developing, checking and validating the various parts of this software. We are very grateful to Steve Bengtson, John Doherty, Maciek Lubczynski, Wolfgang Schäfer, Udo Quek, Axel Voss and Jinhui Zhang who tested the software and provided many valuable comments and criticisms. For their encouragement and support, we thank Ian Callow, Lothar Moosmann, Renate Taugs, Gerrit van Tonder and Ray Volker. The authors also wish to thank Alpha Robinson, a scientist at the University of Paderborn, who checked Chapter 3 of this user's guide. And thanks to our readers

and software users - it is not possible for us to list by name here all the readers and users who have made useful suggestions; we are very grateful for these.

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1. Introduction

The applications of MODFLOW, a modular three-dimensional finite-difference groundwater model of the U. S. Geological Survey, to the description and prediction of the behavior of groundwater systems have increased significantly over the last few years. The “original” version of MODFLOW-88 (McDonald and Harbaugh, 1988) or MODFLOW-96 (Harbaugh and McDonald, 1996a, 1996b) can simulate the effects of wells, rivers, drains, head-dependent boundaries, recharge and evapotranspiration. Since the publication of MODFLOW various codes have been developed by numerous investigators. These codes are called *packages*, *models* or sometimes simply *programs*. *Packages* are integrated with MODFLOW, each package deals with a specific feature of the hydrologic system to be simulated, such as wells, recharge or river. *Models* or *programs* can be stand-alone codes or can be integrated with MODFLOW. A stand-alone model or program communicates with MODFLOW through data files. The advective transport model PMPATH (Chiang and Kinzelbach, 1994, 1998), the solute transport model MT3D (Zheng, 1990), MT3DMS (Zheng and Wang, 1998) and the parameter estimation programs PEST (Doherty et al., 1994) and UCODE (Poeter and Hill, 1998) use this approach. The solute transport model MOC3D (Konikow et al., 1996) and the inverse model MODFLOWP (Hill, 1992) are integrated with MODFLOW. Both codes use MODFLOW as a function for calculating flow fields.

This text and the companion software Processing Modflow for Windows (PMWIN) offer a totally integrated simulation system for modeling groundwater flow and transport processes with MODFLOW-88, MODFLOW-96, PMPATH, MT3D, MT3DMS, MOC3D, PEST and UCODE.

PMWIN comes with a professional graphical user-interface, the supported models and programs and several other useful modeling tools. The graphical user-interface allows you to create and simulate models with ease and fun. It can import DXF- and raster graphics and handle models with up to 1,000 stress periods, 80 layers and 250,000 cells in each model layer. The modeling tools include a **Presentation** tool, a **Result Extractor**, a **Field Interpolator**, a **Field Generator**, a **Water Budget Calculator** and a **Graph Viewer**. The **Result Extractor** allows the user to extract simulation results from any period to a spread sheet. You can then view the results or save them in ASCII or SURFER-compatible data files. Simulation results include hydraulic heads, drawdowns, cell-by-cell flow terms, compaction, subsidence, Darcy velocities, concentrations and mass terms. The **Field Interpolator** takes measurement data and interpolates the data to each model cell. The model grid can be irregularly spaced. The **Water Budget Calculator** not only calculates the budget of user-specified zones but also the exchange of flows between such zones. This facility is very useful in many practical cases. It allows the user to determine the flow through a particular boundary. The **Field Generator** generates fields with

heterogeneously distributed transmissivity or hydraulic conductivity values. It allows the user to statistically simulate effects and influences of unknown small-scale heterogeneities. The **Field Generator** is based on Mejía's (1974) algorithm. The **Graph Viewer** displays temporal development curves of simulation results including hydraulic heads, drawdowns, subsidence, compaction and concentrations.

Using the **Presentation** tool, you can create labelled contour maps of input data and simulation results. You can fill colors to modell cells containing different values and report-quality graphics may be saved to a wide variety of file formats, including SURFER, DXF, HPGL and BMP (Windows Bitmap). The **Presention** tool can even create and display two dimensional animation sequences using the simulation results (calculated heads, drawdowns or concentration).

At present, PMWIN supports seven additional packages, which are integrated with the "original" MODFLOW. They are Time-Variant Specified-Head (CHD1), Direct Solution (DE45), Density (DEN1), Horizontal-Flow Barrier (HFB1), Interbed-Storage (IBS1), Reservoir (RES1) and Streamflow-Routing (STR1). The Time-Variant Specified-Head package (Leake et al., 1991) was developed to allow constant-head cells to take on different values for each time step. The Direct Solution package (Harbaugh, 1995) provides a direct solver using Gaussian elimination with an alternating diagonal equation numbering scheme. The Density package (Schaars and van Gerven, 1997) was designed to simulate the effect of density differences on the groundwater flow system. The Horizontal-Flow Barrier package (Hsieh and Freckleton, 1992) simulates thin, vertical low-permeability geologic features (such as cut-off walls) that impede the horizontal flow of ground water. The Interbed-Storage package (Leake and Prudic, 1991) simulates storage changes from both elastic and inelastic compaction in compressible fine-grained beds due to removal of groundwater. The Reservoir package (Fenske et al., 1996) simulates leakage between a reservoir and an underlying ground-water system as the reservoir area expands and contracts in response to changes in reservoir stage. The Streamflow-Routing package (Prudic, 1988) was designed to account for the amount of flow in streams and to simulate the interaction between surface streams and groundwater.

The particle tracking model PMPATH uses a semi-analytical particle tracking scheme (Pollock, 1988) to calculate the groundwater paths and travel times. PMPATH allows a user to perform particle tracking with just a few clicks of the mouse. Both forward and backward particle tracking schemes are allowed for steady-state and transient flow fields. PMPATH calculates and displays pathlines or flowlines and travel time marks simultaneously. It provides various on-screen graphical options including head contours, drawdown contours and velocity vectors.

The MT3D transport model uses a mixed Eulerian-Lagrangian approach to the solution of the three-dimensional advective-dispersive-reactive transport equation. MT3D is based on the assumption that changes in the concentration field will not affect the flow field significantly. This

allows the user to construct and calibrate a flow model independently. After a flow simulation is complete, MT3D simulates solute transport by using the calculated hydraulic heads and various flow terms saved by MODFLOW. MT3D can be used to simulate changes in concentration of single species miscible contaminants in groundwater considering advection, dispersion and some simple chemical reactions. The chemical reactions included in the model are limited to equilibrium-controlled linear or non-linear sorption and first-order irreversible decay or biodegradation.

MT3DMS is a further development of MT3D. The abbreviation MS denotes the Multi-Species structure for accommodating add-on reaction packages. MT3DMS includes three major classes of transport solution techniques, i.e., the standard finite difference method; the particle tracking based Eulerian-Lagrangian methods; and the higher-order finite-volume TVD method. In addition to the explicit formulation of MT3D, MT3DMS includes an implicit iterative solver based on generalized conjugate gradient (GCG) methods. If this solver is used, dispersion, sink/source, and reaction terms are solved implicitly without any stability constraints.

The MOC3D transport model computes changes in concentration of a single dissolved chemical constituent over time that are caused by advective transport, hydrodynamic dispersion (including both mechanical dispersion and diffusion), mixing or dilution from fluid sources, and mathematically simple chemical reactions, including decay and linear sorption represented by a retardation factor. MOC3D uses the method of characteristics to solve the transport equation on the basis of the hydraulic gradients computed with MODFLOW for a given time step. This implementation of the method of characteristics uses particle tracking to represent advective transport and explicit finite-difference methods to calculate the effects of other processes. For improved efficiency, the user can apply MOC3D to a subgrid of the primary MODFLOW grid that is used to solve the flow equation. However, the transport subgrid must have uniform grid spacing along rows and columns. Using MODFLOW as a built-in function, MOC3D can be modified to simulate density-driven flow and transport.

The purpose of PEST and UCODE is to assist in data interpretation and in model calibration. If there are field or laboratory measurements, PEST and UCODE can adjust model parameters and/or excitation data in order that the discrepancies between the pertinent model-generated numbers and the corresponding measurements are reduced to a minimum. Both codes do this by taking control of the model (MODFLOW) and running it as many times as is necessary in order to determine this optimal set of parameters and/or excitations.

System Requirements

Hardware

Personal computer running Microsoft Windows 95/98 or Windows NT 4.0 or above.
16 MB of available memory (32MB or more highly recommended).
A CD-ROM drive and a hard disk.
VGA or higher-resolution monitor.
Microsoft Mouse or compatible pointing device.

Software

A FORTRAN compiler is required if you intend to modify and compile the models MODFLOW-88, MODFLOW-96, MOC3D, MT3D or MT3DMS. For the reason of compability, the models must be compiled by a **Lahey Fortran** compiler. The source codes of the above-mentioned models are saved in the folder \Source\ of the CD-ROM.

Setting Up PMWIN

You install PMWIN on your computer using the self-installing program PM32010.EXE contained in the folder \programs\pm5\ of the CD-ROM. **Please note:** If you are using Windows NT 4.0, you must install the Service Pack 3 (or above) before installing PMWIN. Refer to the file readme.txt on the PM5 CD-ROM for more information.

Documentation

The folder \Document\ of the CD-ROM contains electronic documents in the Portable Document Format (PDF). You must first install the Acrobat® Reader before you can read or print the PDF documents. You can find the installation file of the Acrobat® Reader in the folder \Reader\. Execute the file \Reader\win95\ar302.exe from the CD directly and follow the screen to install the Reader.

Starting PMWIN

Once you have completed the installation procedure, you can start Processing Modflow by using the **Start** button on the task bar in Windows.

Online Help

The online help system references nearly all aspects of PMWIN. You can access Help through the Help menu Contents command, by searching for specific topics with the Help Search tool, or by clicking the Help button to get context sensitive Help.

Help Search

The fastest way to find a particular topic in Help is to use the **Search** dialog box. To display the **Search** dialog box, either choose Search from the **Help** menu or click the Search button on any **Help** topic screen.

- **To search Help**

1. From the **Help** menu, choose **Search**. (You can also click the **Search** button from any **Help** topic window).
2. In the **Search** dialog box, type a word, or select one from the list by scrolling up or down. Press ENTER or choose Show Topics to display a list of topics related to the word you specified.
3. Select a topic and press ENTER or choose Go To to view the topic.

Context-Sensitive Help

Many parts of the PMWIN Help facility are context-sensitive. Context-sensitive means you can access help on any part of PMWIN directly by clicking the Help button or by pressing the F1 key.

Updates

Today the development of groundwater modeling techniques is progressing very rapidly, and a groundwater model must periodically be updated and expanded. For updates of PMWIN and our other software you may access the following web-pages on the Internet:

http://www.uovs.ac.za/igs/index.htm
http://www.baum.ethz.ch./ihw/soft/welcome.html

FOR YOUR NOTES

2. Your First Groundwater Model with PMWIN

It takes just a few minutes to build your first groundwater flow model with PMWIN. First, create a groundwater model by choosing **New Model** from the **File** menu. Next, determine the size of the model grid by choosing **Mesh Size** from the **Grid** menu. Then, specify the geometry of the model and set the model parameters, such as hydraulic conductivity, effective porosity etc.. Finally, perform the flow simulation by choosing **MODFLOW▸Run...** from the **Models** menu.

After completing the flow simulation, you can use the modeling tools provided by PMWIN to view the results, to calculate water bugdets of particular zones, or graphically display the results, such as head contours. You can also use PMPATH to calculate and save pathlines or use the finite difference transport models MT3D or MOC3D to simulate transport processes.

This chapter provides an overview of the modeling process with PMWIN, describes the basic skills you need to use PMWIN, and takes you step by step through a sample problem. A complete reference for all menus and dialog boxes in PMWIN is contained in Chapter 3. The advective transport model PMPATH and the modeling tools are described in Chapter 4 and Chapter 5, respectively.

Overview of the Sample Problem

As shown in Fig. 2.1, an aquifer system with two stratigraphic units is bounded by no-flow boundaries on the North and South sides. The West and East sides are bounded by rivers, which are in full hydraulic contact with the aquifer and can be considered as fixed-head boundaries. The hydraulic heads on the west and east boundaries are 9 m and 8 m above reference level, respectively.

The aquifer system is unconfined and isotropic. The horizontal hydraulic conductivities of the first and second stratigraphic units are 0.0001 m/s and 0.0005 m/s, respectively. Vertical hydraulic conductivity of both units is assumed to be 10 percent of the horizontal hydraulic conductivity. The effective porosity is 25 percent. The elevation of the ground surface (top of the first stratigraphic unit) is 10m. The thickness of the first and the second units is 4 m and 6 m, respectively. A constant recharge rate of 8×10^{-9} m/s is applied to the aquifer. A contaminated area lies in the first unit next to the west boundary. The task is to isolate the contaminated area using a fully penetrating pumping well located next to the eastern boundary.

A numerical model has to be developed for this site to calculate the required pumping rate of the well. The pumping rate must be high enough, so that the contaminated area lies within the

capture zone of the pumping well. We will use PMWIN to construct the numerical model and use PMPATH to compute the capture zone of the pumping well. Based on the calculated groundwater flow field, we will use MT3D and MOC3D to simulate the contaminant transport. We will show how to use PEST and UCODE to calibrate the flow model and finally we will create an animation sequence displaying the development of the contaminant plume.

To demonstrate the use of the transport models, we assume that the pollutant is dissolved into groundwater at a rate of 1×10^{-4} μg/s/m^2. The longitudinal and transverse dispersivities of the aquifer are 10m and 1m, respectively. The retardation factor is 2. The initial concentration, molecular diffusion coefficient, and decay rate are assumed to be zero. We will calculate the concentration distribution after a simulation time of 3 years and display the breakthrough curves (concentration versus time) at two points [X, Y] = [290, 310], [390, 310] in both units.

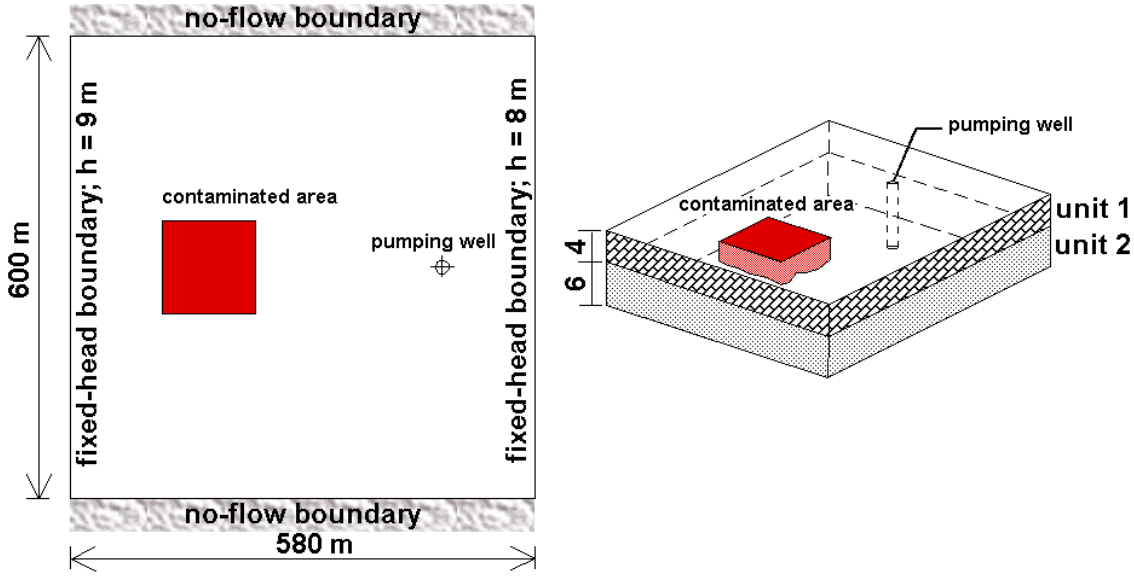


Fig. 2.1 Configuration of the sample problem

2.1 Run a Steady-State Flow Simulation

Six main steps must be performed in a steady-state flow simulation:

1. Create a new model model
2. Assign model data
3. Perform the flow simulation
4. Check simulation results
5. Calculate subregional water budget
6. Produce output

Step 1: Create a New Model

The first step in running a flow simulation is to create a new model.

▸ **To create a new model**

1. Choose **New Model** from the **File** menu. A **New Model** dialog box appears. Select a folder for saving the model data, such as C:\PM5DATA\SAMPLE, and type the file name SAMPLE for the sample model. A model must always have the file extension **.PM5**. All file names valid under Windows 95/98/NT with up to 120 characters can be used. It is a good idea to save every model in a separate folder, where the model and its output data will be kept. This will also allow you to run several models simultaneously (multitasking).
2. Click **OK**.
   PMWIN takes a few seconds to create the new model. The name of the new model name is shown in the title bar.

Step 2: Assign Model Data

The second step in running a flow simulation is to generate the model grid (mesh), specify boundary conditions, and assign model parameters to the model grid.

PMWIN requires the use of **consistent units** throughout the modeling process. For example, if you are using length [L] units of meters and time [T] units of seconds, hydraulic conductivity will be expressed in units of [m/s], pumping rates will be in units of [m^3/s] and dispersivities will be in units of [m].

In MODFLOW, an aquifer system is replaced by a discretized domain consisting of an array of nodes and associated finite difference blocks (cells). Fig. 2.2 shows a spatial discretization of an aquifer system with a mesh of cells and nodes at which hydraulic heads are calculated. The nodal grid forms the framework of the numerical model. Hydrostratigraphic units can be represented by one or more model layers. The thicknesses of each model cell and the width of each column and row may be variable. The locations of cells are described in terms of columns, rows, and layers. PMWIN uses an index notation [J, I, K] for locating the cells. For example, the cell located in the 2nd column, 6th row, and the first layer is denoted by [2, 6, 1].

▸ **To generate the model grid**

1. Choose **Mesh Size** from the **Grid** menu.
   The **Model Dimension** dialog box appears (Fig. 2.3).
2. Enter 3 for the number of layers, 30 for the numbers of columns and rows, and 20 for the size of columns and rows.

The first and second stratigraphic units will be represented by one and two model layers, respectively.

3. Click **OK**.

   PMWIN changes the pull-down menus and displays the generated model grid (Fig. 2.4). PMWIN allows you to shift or rotate the model grid, change the width of each model column or row, or to add/delete model columns or rows. For our sample problem, you do not need to modify the model grid. See section 3.1 for more information about the **Grid Editor**.

4. Choose **Leave Editor** from the **File** menu or click the **leave editor** button  .

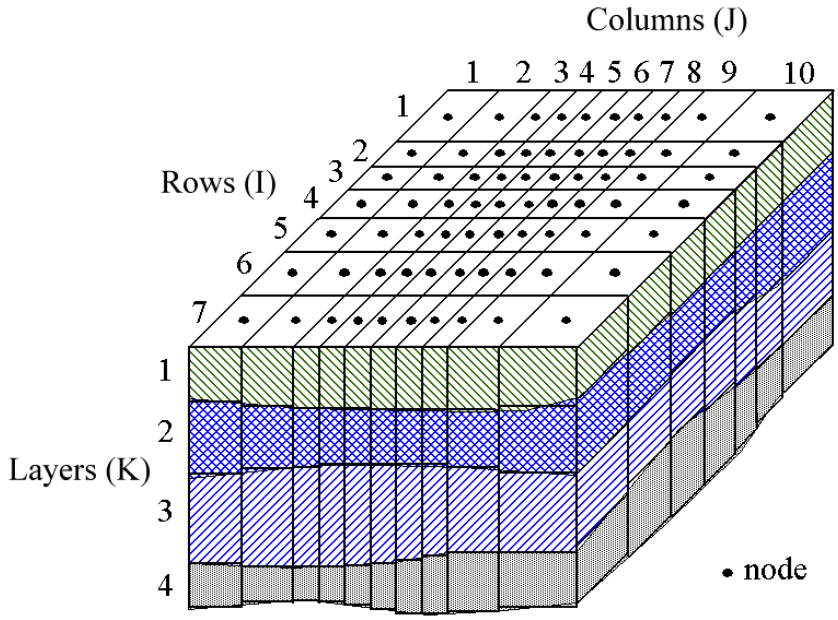


Fig. 2.2 Spatial discretization of an aquifer system and the cell indices

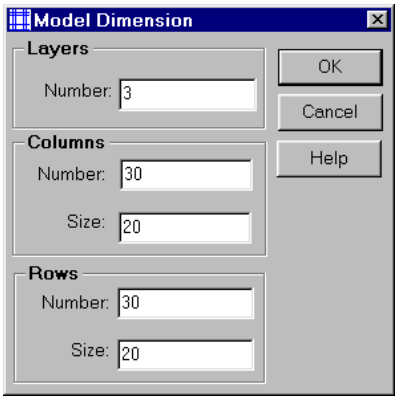


Fig. 2.3 The **Model Dimension** dialog box

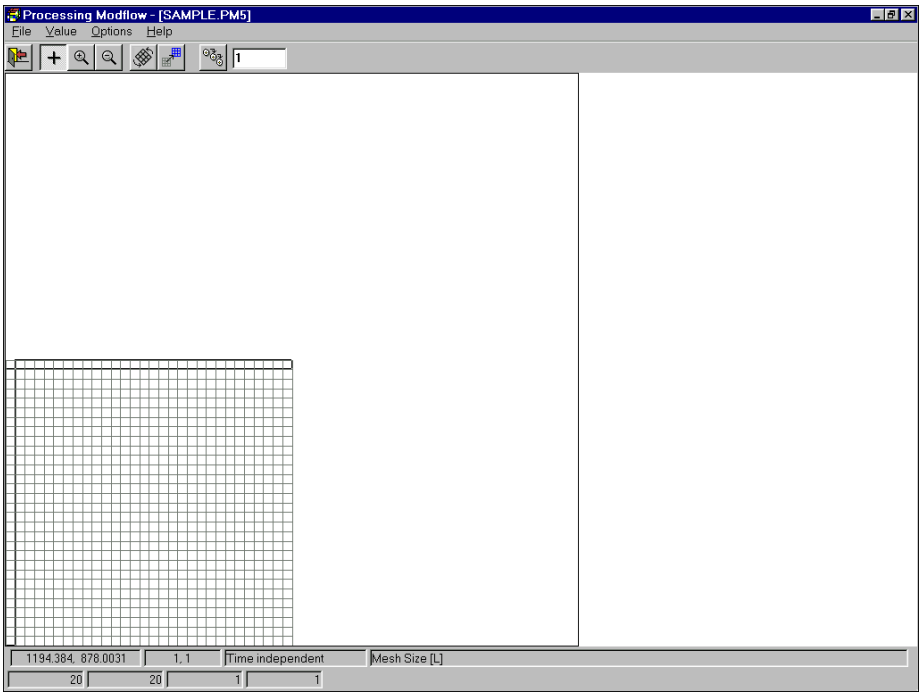


Fig. 2.4 The generated model grid

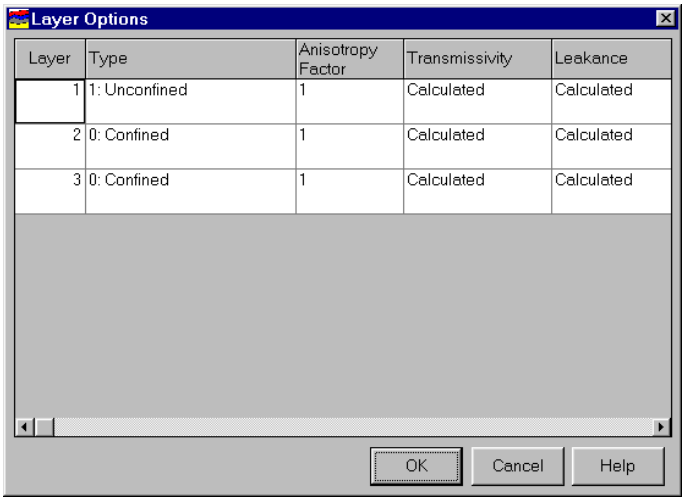


Fig. 2.5 The **Layer Options** dialog box and the layer type drop-down list

The next step is to specify the type of layers.

- **To assign the type of layers**

1. Choose **Layer Type** from the **Grid** menu.
   A **Layer Options** dialog box appears.

2. Click a cell of the **Type** column, a drop-down button will appear within the cell. By clicking the drop-down button, a list containing the avaliable layer types (Fig. 2.5) will be displayed.
3. Select **1: Unconfined** for the first layer and **0: Confined** for the other layers then click **OK** to close the dialog box.

As transmissivity and leakance are - by default - assumed to be calculated (see Fig. 2.5) from conductivities and geometrical properties, the primary input variables to be specified are horizontal and vertical hydraulic conductivities.

Now, you must specify basic boundary conditions of the flow model. The basic boundary contition array (IBOUND array) contains a code for each model cell which indicates whether (1) the hydraulic head is computed (active variable-head cell or active cell), (2) the hydraulic head is kept fixed at a given value (fixed-head cell or time-varying specified-head cell), or (3) no flow takes place within the cell (inactive cell). Use 1 for an active cell, -1 for a constant-head cell, and 0 for an inactive cell. For the sample problem, we need to assign -1 to the cells on the west and east boundaries and 1 to all other cells.

▸ **To assign the boundary condition to the flow model**

1. Choose **Boundary Condition ▸ IBOUND (Modflow)** from the **Grid** Menu.
   The **Data Editor** of PMWIN appears with a plan view of the model grid (Fig. 2.6). The grid cursor is located at the cell [1, 1, 1], that is the upper-left cell of the first layer. The value of the current cell is shown at the bottom of the status bar. The default value of the IBOUND array is 1. The grid cursor can be moved horizontally by using the arrow keys or by clicking the mouse on the desired position. To move to an other layer, use PgUp or PgDn keys or click the edit field in the tool bar, type the new layer number, and then press enter.

Note that a DXF-map is loaded by using the Maps Options. See Chapter 3 for details.

2. Press the *right* mouse button. PMWIN shows a **Cell Value** dialog box.
3. Type -1 in the dialog box, then click **OK**.
   The upper-left cell of the model has been specified to be a fixed-head cell.
4. Now turn on duplication by clicking the **duplication** button  .
   Duplication is on, if the relief of the **duplication** button is sunk. The current cell value will be duplicated to all cells passed by the grid cursor, if it is moved while duplication is on. You can turn off duplication by clicking the **duplication** button again.
5. Move the grid cursor from the upper-left cell [1, 1, 1] to the lower-left cell [1, 30, 1] of the model grid.

The value of -1 is duplicated to all cells on the west side of the model.

6. Move the grid cursor to the upper-right cell [30, 1, 1].
7. Move the grid cursor from the upper-right cell [30, 1, 1] to the lower-right cell [30, 30, 1].
   The value of -1 is duplicated to all cells on the east side of the model.
8. Turn on **layer copy** by clicking the **layer copy** button  .
   Layer copy is on, if the relief of the **layer copy** button is sunk. The cell values of the current layer will be copied to other layers, if you move to the other model layer while layer copy is on. You can turn off layer copy by clicking the **layer copy** button again.
9. Move to the second layer and then to the third layer by pressing the PgDn key twice.
   The cell values of the first layer are copied to the second and third layers.
10. Choose **Leave Editor** from the **File** menu or click the **leave editor** button  .

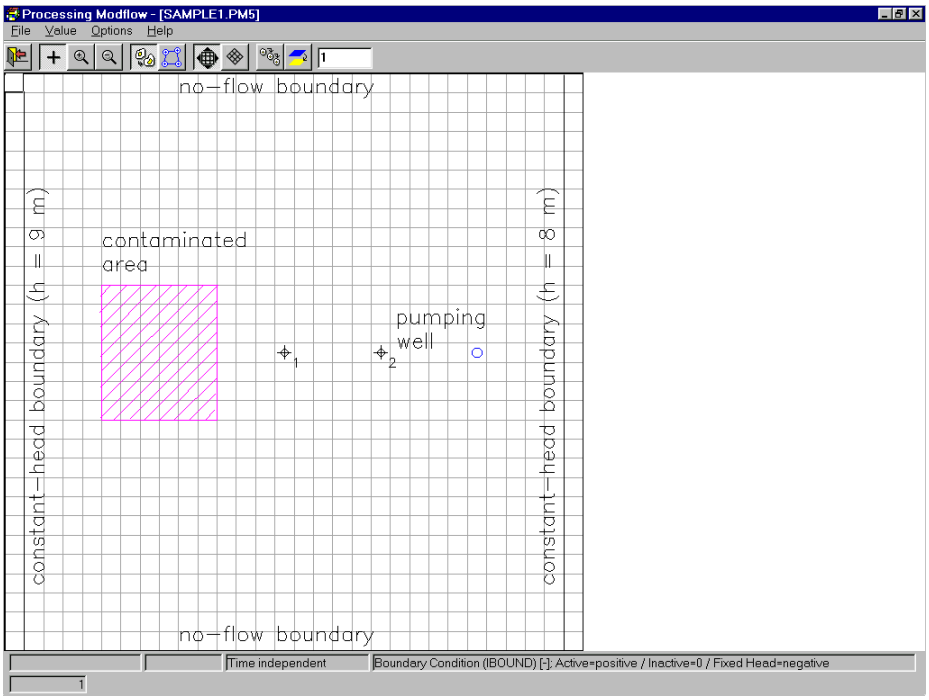


Fig. 2.6 Data Editor with a plan view of the model grid.

The next step is to specify the geometry of the model.

▸ **To specify the elevation of the top of model layers**

1. Choose **Top of Layers (TOP)** from the **Grid** menu.
   PMWIN displays the model grid.
2. Choose **Reset Matrix...** from the **Value** menu (or press Ctrl+R).
   A **Reset Matrix** dialog box appears.
3. Enter 10 in the dialog box, then click **OK**.

The elevation of the top of the first layer is set to 10.

4. Move to the second layer by pressing PgDn.
5. Repeat steps 2 and 3 to set the top elevation of the second layer to 6 and the top elevation of the third layer to 3.
6. Choose **Leave Editor** from the **File** menu or click the **leave editor** button  .

▸ **To specify the elevation of the bottom of model layers**

1. Choose **Bottom of Layers (BOT)** from the **Grid** menu.
2. Repeat the same procedure as described above to set the bottom elevation of the first, second and third layers to 6, 3 and 0, respectively.
3. Choose **Leave Editor** from the **File** menu or click the **leave editor** button  .

We are going to specify the temporal and spatial parameters of the model. The spatial parameters for sample problem include the initial hydraulic head, horizontal and vertical hydraulic conductivities and effective porosity.

▸ **To specify the temporal parameters**

1. Choose **Time...** from the **Parameters** menu.
   A **Time Parameters** dialog box will come up. The temporal parameters include the time unit and the numbers of stress periods, time steps and transport steps. In MODFLOW, the simulation time is divided into stress periods - i.e., time intervals during which all external excitations or stresses are constant - which are, in turn, divided into time steps. In most transport models, each flow time step is further divided into smaller transport steps. The length of stress periods is not relevant to a steady state flow simulation. However, as we want to perform contaminant transport simulation with MT3D and MOC3D, the actual time length must be specified in the table.
2. Enter 9.46728E+07 (seconds) for **Length** of the first period.
3. Click **OK** to accept the other default values.

Now, you need to specify the initial hydraulic head for each model cell. The initial hydraulic head at a fixed-head boundary will be kept constant during the flow simulation. The other heads are starting values in a transient simulation or first guesses for the iterative solver in a steady-state simulation. Here we firstly set all values to 8 and then correct the values on the west side by overwriting them with a value of 9.

▸ **To specify the initial hydraulic head**

1. Choose **Initial Hydraulic Heads** from the **Parameters** menu.
   PMWIN displays the model grid.
2. Choose **Reset Matrix...** from the **Value** menu (or press Ctrl+R) and enter 8 in the dialog box, then click **OK**.
3. Move the grid cursor to the upper-left model cell.
4. Press the *right* mouse button and enter 9 into the **Cell Value** dialog box, then click **OK**.
5. Now turn on **duplication** by clicking the **duplication** button  .
   Duplication is on, if the relief of the **duplication** button is sunk. The current cell value will be duplicated to all cells passed over by the grid cursor, if **duplication** is on.
6. Move the grid cursor from the upper-left cell to the lower-left cell of the model grid.
   The value of 9 is duplicated to all cells on the west side of the model.
7. Turn on **layer copy** by clicking the **layer copy** button  .
   Layer copy is on, if the relief of the **layer copy** button is sunk. The cell values of the current layer will be copied to another layer, if you move to the other model layer while **layer copy** is on.
8. Move to the second layer and the third layer by pressing PgDn twice.
   The cell values of the first layer are copied to the second and third layers.
9. Choose **Leave Editor** from the **File** menu or click the **leave editor** button  .

▸ **To specify the horizontal hydraulic conductivity**

1. Choose **Horizontal Hydraulic Conductivity** from the **Parameters** menu.
2. Choose **Reset Matrix...** from the **Value** menu (or press Ctrl+R), type 0.0001 in the dialog box, then click **OK**.
3. Move to the second layer by pressing PgDn.
4. Choose **Reset Matrix...** from the **Value** menu (or press Ctrl+R), type 0.0005 in the dialog box, then click **OK**.
5. Repeat steps 3 and 4 to set the value of the third layer to 0.0005.
6. Choose **Leave Editor** from the **File** menu or click the **leave editor** button  .

▸ **To specify the vertical hydraulic conductivity**

1. Choose **Vertical Hydraulic Conductivity** from the **Parameters** menu.
2. Choose **Reset Matrix...** from the **Value** menu (or press Ctrl+R), type 0.00001 in the dialog box, then click **OK**.
3. Move to the second layer by pressing PgDn.
4. Choose **Reset Matrix...** from the **Value** menu (or press Ctrl+R), type 0.00005 in the dialog

box, then click **OK**.

5. Repeat steps 3 and 4 to set the value of the third layer to 0.00005.
6. Choose **Leave Editor** from the **File** menu or click the **leave editor** button  .

▸ **To specify the effective porosity**

1. Choose **Effective Porosity** from the **Parameters** menu.
   Because the standard value is the same as the prescribed value of 0.25, you may leave the editor and save the changes.
2. Choose **Leave Editor** from the **File** menu or click the **leave editor** button  .

▸ **To specify the recharge rate**

1. Choose **MODFLOW▸ Recharge** from the **Models** menu.
2. Choose **Reset Matrix...** from the **Value** menu (or press Ctrl+R), enter 8E-9 for **Recharge Flux [L/T]** in the dialog box, then click **OK**.
3. Choose **Leave Editor** from the **File** menu or click the **leave editor** button  .

The last step before performing the flow simulation is to specify the location of the pumping well and its pumping rate. In MODFLOW, an injection or pumping well is represented by a node (or a cell). The user specifies an injection or pumping rate for each node. It is implicitly assumed that the well penetrates the full thickness of the cell. MODFLOW can simulate the effects of pumping from a well that penetrates more than one aquifer or layer provided that the user supplies the pumping rate for each layer. The total pumping rate for the multilayer well is equal to the sum of the pumping rates from the individual layers. The pumping rate for each layer (Q_k) can be approximately calculated by dividing the total pumping rate (Q_{total}) in proportion to the layer transmissivities (McDonald and Harbaugh, 1988):

$$Q_k = Q_{total} \cdot \frac{T_k}{\Sigma T} \qquad (2.1)$$

where T_k is the transmissivity of layer k and ΣT is the sum of the transmissivities of all layers penetrated by the multilayer well. Unfortunately, as the first layer is unconfined, we do not exactly know the saturated thickness and the transmissivity of this layer at the position of the well. Eq. 2.1 cannot be used unless we assume a saturated thickness for calculating the transmissivity. An other possibility to simulate a multi-layer well is to set a very large vertical hydraulic conductivity (or vertical leakance), e.g. 1 m/s, to all cells of the well. The total pumping rate is assigned to the lowest cell of the well. For the display purpose, a very small pumping rate (say, 1×10^{-10} m^3/s) can be assigned to other cells of the well. In this way, the exact

extraction rate from each penetrated layer will be calculated by MODFLOW implicitly and the value can be obtained by using the **Water Budget Calculator** (see below).

As we do not know the required pumping rate for capturing the contaminated area shown in Fig. 2.1, we will try a total pumping rate of 0.0012 m^3/s.

▸ **To specify the pumping well and the pumping rate**

1. Choose **MODFLOW▸Well** from the **Models** menu.
2. Move the grid cursor to the cell [25, 15, 1]
3. Press the right mouse button and type -1E-10, then click **OK**. Note that a negative value is used to indicate a *pumping* well.
4. Move to the second layer by pressing PgDn.
5. Press the right mouse button and type -1E-10 then click **OK**.
6. Move to the third layer by pressing PgDn.
7. Press the right mouse button and type -0.0012 then click **OK**.
8. Choose **Leave Editor** from the **File** menu or click the **leave editor** button  .

Step 3: Perform the Flow Simulation

▸ **To perform the flow simulation**

1. Choose **MODFLOW▸Run...** from the **Models** menu.
   The **Run Modflow** dialog box appears (Fig. 2.7).
2. Click **OK** to start the flow computation.
   Prior to running MODFLOW, PMWIN will use the user-specified data to generate input files for MODFLOW (and optionally MODPATH) as listed in the table of the **Run Modflow** dialog box. An input file will be generated only if the **generate** flag is set to ☒. You can click on the button to toggle the **generate** flag between ☒ and ☐. Generally, you do not need to change the flags, as PMWIN will care about the settings.

Step 4: Check Simulation Results

During a flow simulation, MODFLOW writes a detailed run record to the listing file *path*\OUTPUT.DAT, where *path* is the folder in which your model data are saved. If a flow simulation is successfully completed, MODFLOW saves the simulation results in various unformatted (binary) files as listed in Table 2.1. Prior to running MODFLOW, the user may control the output of these unformatted (binary) files by choosing **Modflow▸Output Control** from the **Models** menu. The output file *path*\INTERBED.DAT will only be generated, if the Interbed Storage Package is activated (see Chapter 3 for details about the Interbed Storage Package).

To check the quality of the simulation results, MODFLOW calculates a volumetric water budget for the entire model at the end of each time step, and saves it in the file output.dat (see Table 2.2). A water budget provides an indication of the overall acceptability of the numerical solution. In numerical solution techniques, the system of equations solved by a model actually consists of a flow continuity statement for each model cell. Continuity should also exist for the total flows into and out of the entire model or a sub-region. This means that the difference between total inflow and total outflow should equal to 0 (steady-state flow simulation) or to the total change in storage (transient flow simulation). It is recommended to check the record file or at least take a glance at it. The record file contains other further essential information. In case of difficulties, this supplementary information could be very helpful.

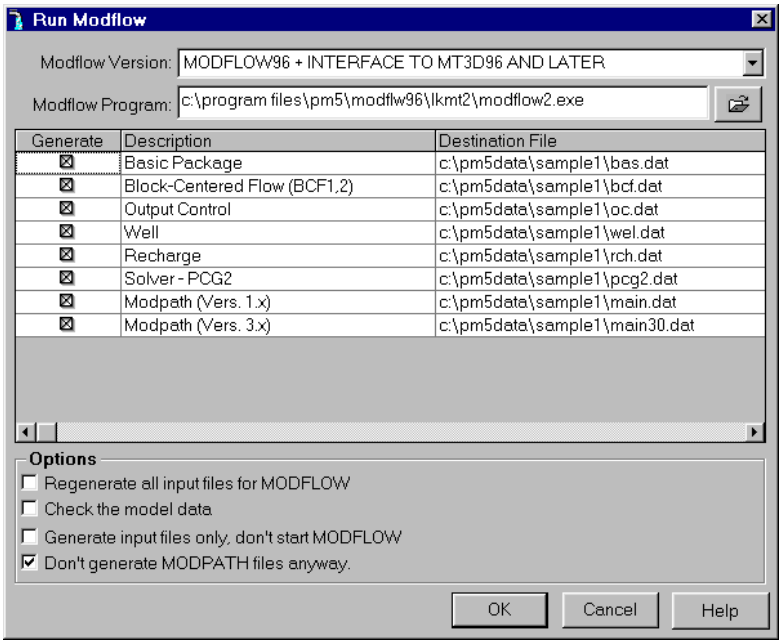


Fig. 2.7 The **Run Modflow** dialog box

Table 2.1 Output files from MODFLOW

File	Contents
path\OUTPUT.DAT	Detailed run record and simulation report
path\HEADS.DAT	Hydraulic heads
path\DDOWN.DAT	Drawdowns, the difference between the starting heads and the calculated hydraulic heads.
path\BUDGET.DAT	Cell-by-Cell flow terms
path\INTERBED.DAT	Subsidence of the entire aquifer and compaction and preconsolidation heads in individual layers.
path\MT3D.FLO	Interface file to MT3D/MT3DMS. This file is created by the LKMT package provided by MT3D/MT3DMS (Zheng, 1990, 1998).

- *path* is the folder in which the model data are saved.

Table 2.2 Volumetric budget for the entire model written by MODFLOW

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

    CUMULATIVE VOLUMES      L**3       RATES FOR THIS TIME STEP      L**3/T
    ------------------                 ------------------------

          IN:                                   IN:
          ---                                   ---
      CONSTANT HEAD =      209690.3590         CONSTANT HEAD =       2.2150E-03
              WELLS =           0.0000                 WELLS =           0.0000
           RECHARGE =      254472.9380              RECHARGE =       2.6880E-03

           TOTAL IN =      464163.3130              TOTAL IN =       4.9030E-03

         OUT:                                  OUT:
         ----                                  ----
      CONSTANT HEAD =      350533.6880         CONSTANT HEAD =       3.7027E-03
              WELLS =      113604.0310                 WELLS =       1.2000E-03
           RECHARGE =           0.0000              RECHARGE =           0.0000

          TOTAL OUT =      464137.7190             TOTAL OUT =       4.9027E-03

           IN - OUT =          25.5938              IN - OUT =       2.7008E-07

 PERCENT DISCREPANCY =           0.01     PERCENT DISCREPANCY =           0.01
```

Step 5: Calculate subregional water budget

There are situations in which it is useful to calculate water budgets for various subregions of the model. To facilitate such calculations, flow terms for individual cells are saved in the file *path*\BUDGET.DAT. These individual cell flows are referred to as cell-by-cell flow terms, and are of four types: (1) cell-by-cell stress flows, or flows into or from an individual cell due to one of the external stresses (excitations) represented in the model, e.g., pumping well or recharge; (2) cell-by-cell storage terms, which give the rate of accumulation or depletion of storage in an

individual cell; (3) cell-by-cell constant-head flow terms, which give the net flow to or from individual fixed-head cells; and (4) internal cell-by-cell flows, which are the flows across individual cell faces-that is, between adjacent model cells. The **Water Budget Calculator** uses the cell-by-cell flow terms to compute water budgets for the entire model, user-specified subregions, and flows between adjacent subregions.

▸ **To calculate subregional water budget**s

1. Choose **Water Budget** from the **Tools** menu.
   A **Water Budget** dialog box appears (Fig. 2.8). For a steady-state flow simulation, you do not need to change the settings in the **Time** group.
2. Click **Zones**.
   A zone is a subregion of a model for which a water budget will be calculated. A zone is indicated by a zone number ranging from 0 to 50. A zone number must be assigned to each model cell. The zone number 0 indicates that a cell is not associated with any zone. Follow steps 3 to 5 to assign zone numbers 1 to the first and 2 to the second layer.
3. Choose **Reset Matrix...** from the **Value** menu, type 1 in the dialog box, then click **OK**.
4. Press PgDn to move to the second layer.
5. Choose **Reset Matrix...** from the **Value** menu, type 2 in the dialog box, then click **OK**.
6. Choose **Leave Editor** from the **File** menu or click the **leave editor** button .
7. Click **OK** in the **Water Budget** dialog box.

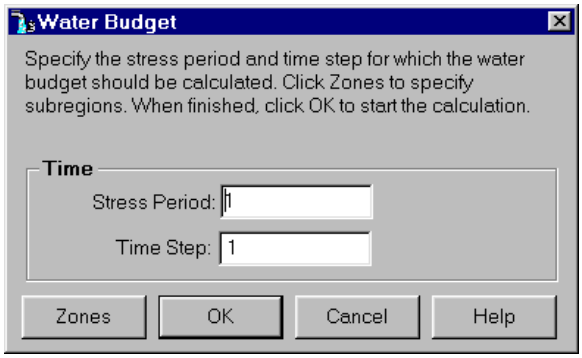


Fig. 2.8 The **Water Budget** dialog box

PMWIN calculates and saves the flows in the file *path*\WATERBDG.DAT as shown in Table 2.3. The unit of the flows is [L^3T^{-1}]. Flows are calculated for each zone in each layer and each time step. Flows are considered **IN**, if they are entering a zone. Flows between subregions are given in a **Flow Matrix**. HORIZ. EXCHANGE gives the flow rate horizontally across the boundary of a zone. EXCHANGE (UPPER) gives the flow rate coming from (**IN**) or going to (**OUT**) to the upper adjacent layer. EXCHANGE (LOWER) gives the flow rate coming from

(**IN**) or going to (**OUT**) to the lower adjacent layer. For example, consider EXCHANGE (LOWER) of ZONE=1 and LAYER=1, the flow rate from the first layer to the second layer is 2.587256E-03 m^3/s. The percent discrepancy in Table 2.3 is calculated by

$$\frac{100 \cdot (IN - OUT)}{(IN + OUT)/2} \tag{2.2}$$

Table 2.3 Output from the Water Budget Calculator

```
FLOWS ARE CONSIDERED "IN" IF THEY ARE ENTERING A SUBREGION
THE UNIT OF THE FLOWS IS [L^3/T]

 TIME STEP    1 OF STRESS PERIOD    1

  ZONE=  1  LAYER=  1
        FLOW TERM              IN             OUT          IN-OUT
          STORAGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
    CONSTANT HEAD  1.8407618E-04  2.4361895E-04 -5.9542770E-05
  HORIZ. EXCHANGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
 EXCHANGE (UPPER)  0.0000000E+00  0.0000000E+00  0.0000000E+00
 EXCHANGE (LOWER)  0.0000000E+00  2.5872560E-03 -2.5872560E-03
            WELLS  0.0000000E+00  1.0000000E-10 -1.0000000E-10
           DRAINS  0.0000000E+00  0.0000000E+00  0.0000000E+00
         RECHARGE  2.6880163E-03  0.0000000E+00  2.6880163E-03
                .              .              .              .
                .              .              .              .
 SUM OF THE LAYER  2.8720924E-03  2.8308749E-03  4.1217543E-05
                .              .              .              .
                .              .              .              .
  ZONE=  2  LAYER=  2
        FLOW TERM              IN             OUT          IN-OUT
          STORAGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
    CONSTANT HEAD  1.0027100E-03  1.7383324E-03 -7.3562248E-04
  HORIZ. EXCHANGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
 EXCHANGE (UPPER)  2.5872560E-03  0.0000000E+00  2.5872560E-03
 EXCHANGE (LOWER)  0.0000000E+00  1.8930938E-03 -1.8930938E-03
            WELLS  0.0000000E+00  1.0000000E-10 -1.0000000E-10
           DRAINS  0.0000000E+00  0.0000000E+00  0.0000000E+00
         RECHARGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
                .              .              .              .
                .              .              .              .
 SUM OF THE LAYER  3.5899659E-03  3.6314263E-03 -4.1460386E-05
-------------------------------------------------------------
                .              .              .              .
                .              .              .              .
WATER BUDGET OF SELECTED ZONES:
                               IN             OUT          IN-OUT
       ZONE(  1):  2.8720924E-03  2.8308751E-03  4.1217310E-05
       ZONE(  2):  3.5899659E-03  3.6314263E-03 -4.1460386E-05
-------------------------------------------------------------

WATER BUDGET OF THE WHOLE MODEL DOMAIN:
        FLOW TERM              IN             OUT          IN-OUT
          STORAGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
    CONSTANT HEAD  2.2149608E-03  3.7026911E-03 -1.4877303E-03
            WELLS  0.0000000E+00  1.2000003E-03 -1.2000003E-03
           DRAINS  0.0000000E+00  0.0000000E+00  0.0000000E+00
         RECHARGE  2.6880163E-03  0.0000000E+00  2.6880163E-03
                .              .              .              .
                .              .              .              .
-------------------------------------------------------------
              SUM  4.9029770E-03  4.9026916E-03  2.8545037E-07
  DISCREPANCY [%]  0.01

The value of the element (i,j) of the following flow matrix gives the flow
rate from the i-th zone into the j-th zone. Where i is the column
index and j is the row index.

FLOW MATRIX:
            1           2
 ..........................
0  1   0.0000      0.0000
0  2   2.5873E-03  0.0000
```

In this example, the percent discrepancy of in- and outflows for the model and each zone in each layer is acceptably small. This means the model equations have been correctly solved.

To calculate the exact flow rates to the well, we repeat the previous procedure for calculating subregional water budgets. This time we only assign the cell [25, 15, 1] to zone 1, the cell [25, 15, 2] to zone 2 and the cell [25, 15, 3] to zone 3. All other cells are assigned to zone 0. The water budget is shown in Table 2.4. The pumping well is extracting 7.7992809E-05 m^3/s from the first layer, 5.603538E-04 m^3/s from the second layer and 5.5766129E-04 m^3/s from the third layer. Almost all water withdrawn comes from the second stratigraphic unit, as can be expected from the configuration of the aquifer.

Table 2.4 Output from the **Water Budget Calculator** for the pumping well

```
FLOWS ARE CONSIDERED "IN" IF THEY ARE ENTERING A SUBREGION
THE UNIT OF THE FLOWS IS [L^3/T]

 TIME STEP    1 OF STRESS PERIOD    1
  ZONE=  1  LAYER=  1
        FLOW TERM              IN             OUT          IN-OUT
          STORAGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
    CONSTANT HEAD  0.0000000E+00  0.0000000E+00  0.0000000E+00
  HORIZ. EXCHANGE  7.7992809E-05  0.0000000E+00  7.7992809E-05
 EXCHANGE (UPPER)  0.0000000E+00  0.0000000E+00  0.0000000E+00
 EXCHANGE (LOWER)  0.0000000E+00  7.9696278E-05 -7.9696278E-05
            WELLS  0.0000000E+00  1.0000000E-10 -1.0000000E-10
           DRAINS  0.0000000E+00  0.0000000E+00  0.0000000E+00
         RECHARGE  3.1999998E-06  0.0000000E+00  3.1999998E-06
                .              .              .              .
                .              .              .              .
 SUM OF THE LAYER  8.1192811E-05  7.9696380E-05  1.4964317E-06
                .              .              .              .
                .              .              .              .
  ZONE=  2  LAYER=  2
        FLOW TERM              IN             OUT          IN-OUT
          STORAGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
    CONSTANT HEAD  0.0000000E+00  0.0000000E+00  0.0000000E+00
  HORIZ. EXCHANGE  5.6035380E-04  0.0000000E+00  5.6035380E-04
 EXCHANGE (UPPER)  7.9696278E-05  0.0000000E+00  7.9696278E-05
 EXCHANGE (LOWER)  0.0000000E+00  6.4027577E-04 -6.4027577E-04
            WELLS  0.0000000E+00  1.0000000E-10 -1.0000000E-10
                .              .              .              .
                .              .              .              .
 SUM OF THE LAYER  6.4005010E-04  6.4027589E-04 -2.2578752E-07


  ZONE=  3  LAYER=  3
        FLOW TERM              IN             OUT          IN-OUT
          STORAGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
    CONSTANT HEAD  0.0000000E+00  0.0000000E+00  0.0000000E+00
  HORIZ. EXCHANGE  5.5766129E-04  0.0000000E+00  5.5766129E-04
 EXCHANGE (UPPER)  6.4027577E-04  0.0000000E+00  6.4027577E-04
 EXCHANGE (LOWER)  0.0000000E+00  0.0000000E+00  0.0000000E+00
            WELLS  0.0000000E+00  1.2000001E-03 -1.2000001E-03
                .              .              .              .
                .              .              .              .
 SUM OF THE LAYER  1.1979371E-03  1.2000001E-03 -2.0629959E-06
```

Step 6: Produce Output

In addition to the water budget, PMWIN provides various possibilities for checking simulation

results and creating graphical outputs. Pathlines and velocity vectors can be displayed by **PMPATH**. Using the **Results Extractor**, simulation results of any layer and time step can be read from the unformatted (binary) result files and saved in *ASCII Matrix* files. An ASCII Matrix file contains a value for each model cell in a layer. PMWIN can load ASCII matrix files into a model grid. The format of the ASCII Matrix file is described in Appendix 2. In the following, we will carry out the steps:

1. Use the **Results Extractor** to read and save the calculated hydraulic heads.
2. Generate a contour map based on the calculated hydraulic heads for the first layer.
3. Use **PMPATH** to compute pathlines as well as the capture zone of the pumping well.

▸ **To read and save the calculated hydraulic heads**

1. Choose **Results Extractor...** from the **Tools** menu
   The **Results Extractor** dialog box appears (Fig. 2.9). The options in the **Results Extractor** dialog box are grouped under four tabs - MODFLOW, MOC3D, MT3D and MT3DMS. In the MODFLOW tab, you may choose a result type from the **Result Type** drop-down box. You may specify the **layer**, **stress period** and **time step** from which the result should be read. The spreadsheet displays a series of columns and rows. The intersection of a row and column is a cell. Each cell of the spreadsheet corresponds to a model cell in a layer. Refer to Chap. 5 for more detailed information about the **Results Extractor**. For the current sample problem, follow steps 2 to 6 to save the hydraulic heads of each layer in three ASCII Matrix files.
2. Choose **Hydraulic Head** from the **Result Type** drop-down box.
3. Type 1 in the **Layer** edit field.
   For the current problem (steady-state flow simulation with only one stress period and one time step), the stress period and time step number should be 1.
4. Click **Read**.
   Hydraulic heads in the first layer at time step 1 and stress period 1 will be read and put into the spreadsheet. You can scroll the spreadsheet by clicking on the scrolling bars next to the spreadsheet.
5. Click **Save**.
   A **Save Matrix As** dialog box appears. By setting the **Save as type** option, the result can be optionally saved as an ASCII matrix or a SURFER data file. Specify the file name H1.DAT and select a folder in which H1.DAT should be saved. Click **OK** when ready.
6. Repeat steps 3, 4 and 5 to save the hydraulic heads of the second and third layer in the files H2.DAT and H3.DAT, respectively.
7. Click **Close** to close the dialog box.

▸ **To generate contour maps of the calculated heads**

1. Choose **Presentation** from the **Tools** menu
   Data specified in **Presentation** will not be used by any parts of PMWIN. We can use **Presentation** to save temporary data or to display simulation results graphically.
2. Choose **Matrix...** from the **Value** menu (or Press Ctrl+B).
   The **Browse Matrix** dialog box appears (Fig. 2.10). Each cell of the spreadsheet corresponds to a model cell in the current layer. You can load an ASCII Matrix file into the spreadsheet or save the spreadsheet in an ASCII Matrix file by clicking **Load** or **Save**. Alternatively, you may select the **Results Extractor** from the **Value** menu, read the head results and use an additional **Apply** button in the **Results Extractor** dialog box to put the data into the **Presentation** matrix.
3. Click the **Load...** button.
   The **Load Matrix** dialog box appears (Fig. 2.11).
4. Click  and select the file H1.DAT, which was saved earlier by the **Results Extractor.** Click **OK** when ready. H1.DAT is loaded into the spreadsheet.
5. In the **Browse Matrix** dialog box, click **OK**.
   The **Browse Matrix** dialog box is closed.
6. Choose **Environment** from the **Options** menu (or Press Ctrl+E).
   The **Environment Options** dialog box appears (Fig. 2.12). The options in the **Environment Options** dialog box are grouped under three tabs. **Appearance** and **Coordinate System** allow the user to modify the appearance and position of the model grid. Use **Contours** to generate contour maps.
7. Click the **Contours** tab, check **Visible**, then click the **Restore Defaults** button.
   Clicking on the **Restore Defaults** button, PMWIN sets the number of contour lines to 11 and uses the maxmum and minimum values in the current layer as the minimum and maximum contour levels (Fig. 2.13). If **Fill Contours** is checked, the contours will be filled with the colors given in the **Fill** column of the table. Use **Label Format** button to specify an appropriate format.

Note that PMWIN will clear the **Visible** check box when you leave the Editor.

8. In the **Environment Options** dialog box, Click **OK**.
   PMWIN will redraw the model and display the contours (Fig. 2.14).
9. To save or print the graphics, choose **Save Plot As...** or **Print Plot...** from the **File** menu.
10. Press PgDn to move to the second layer. Repeat steps 2 to 9 to load the file H2.DAT, display and save the plot.
11. Choose **Leave Editor** from the **File** menu or click the leave editor button  and click **Yes**

to save changes to **Presentation**.

Using the procedure described above, you can generate contour maps based of your input data, any kind of simulation results or any data saved as an ASCII Matrix file. For example, you can create a contour map of the starting heads or you can use the **Result Extractor** to read the concentration distribution and display the contours. You can also generate contour maps of the fields created by the **Field Interpolator** or **Field Generator**. See chapter 5 for details about the Field Interpolator and Field Generator.

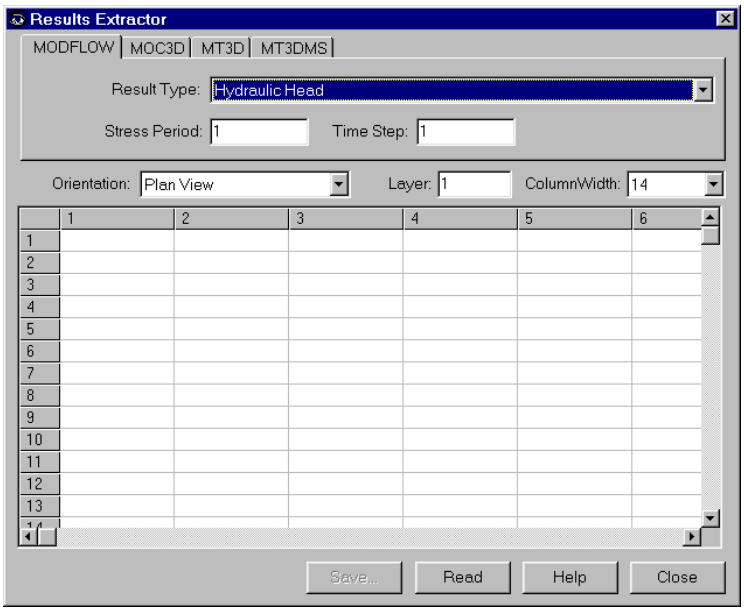


Fig. 2.9 The **Results Extractor** dialog box.

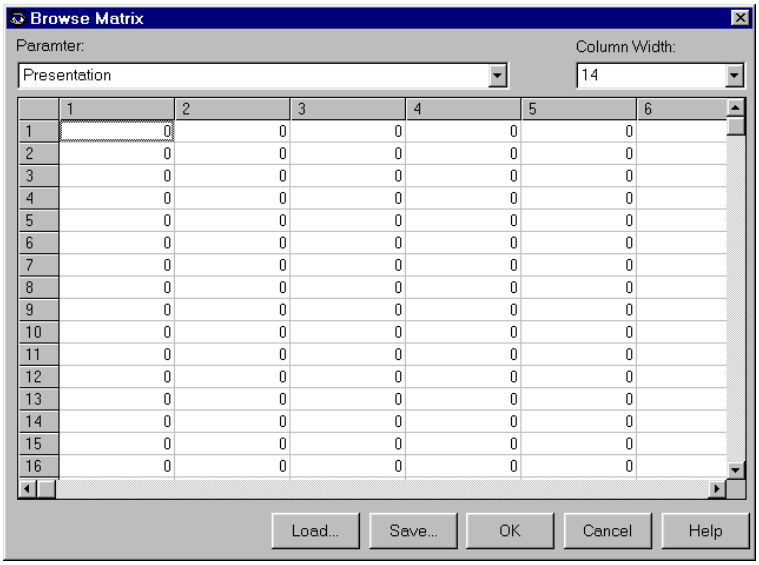


Fig. 2.10 The **Browse Matrix** dialog box

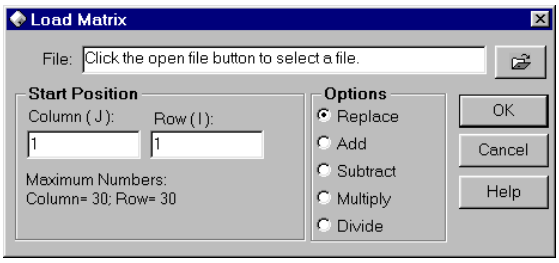


Fig. 2.11 The **Load Matrix** dialog box

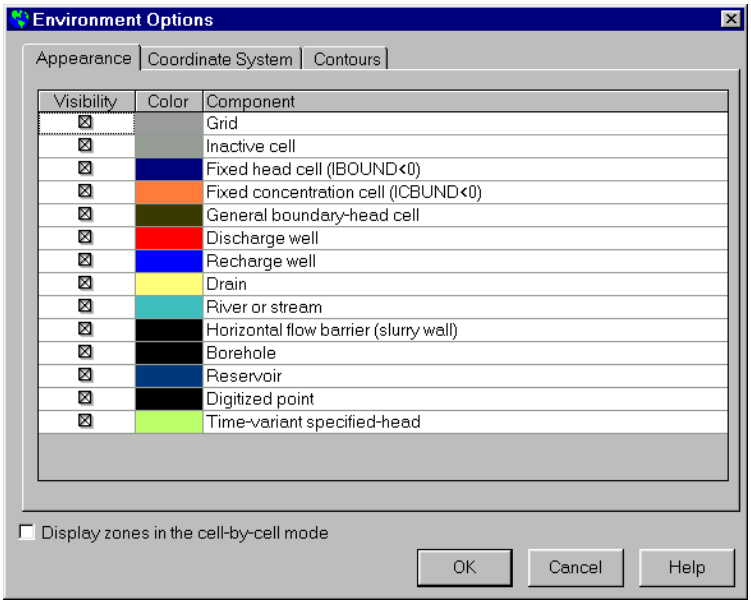


Fig. 2.12 The **Environment Options** dialog box

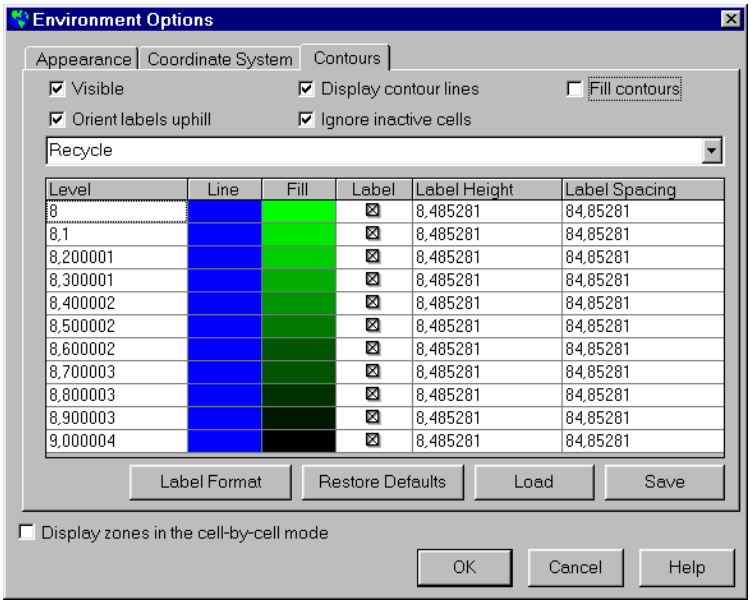


Fig. 2.13 The **Contours** options of the **Environment Options** dialog box

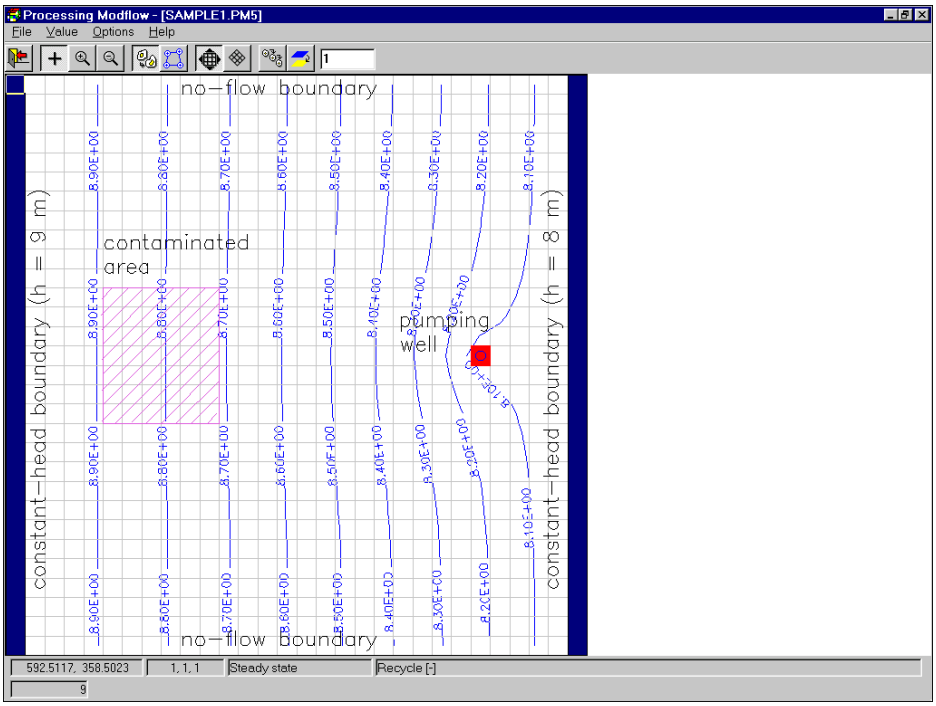


Fig. 2.14 A contour map of the hydraulic heads in the first layer

- **To delineate the capture zone of the pumping well**

1. Choose **PMPATH (Pathlines and Contours)** from the **Models** menu.
   PMWIN calls the advective transport model PMPATH and the current model will be loaded into PMPATH automatically. PMPATH uses a "grid cursor" to define the column and row for which the cross-sectional plots should be displayed. You can move the grid cursor by holding down the Ctrl-key and click the left mouse button on the desired position.

Note that if you subsequently modify and calculate a model within PMWIN, you must load the modified model into PMPATH again to ensure that the modifications can be recognized by PMPATH. To load a model, click  and select a model file with the extension **.PM5** from the **Open Model** dialog box.

2. To calculate the capture zone of the pumping well:
   a. Click the **Set Particle** button 
   b. Move the mouse cursor to the model area. The mouse cursor turns into crosshairs.
   c. Place the crosshairs at the upper-left corner of the pumping well, as shown in Fig. 2.15.
   d. Hold down the left moust button and drag the crosshairs until the window covers the pumping well.
   e. Release the left mouse button.

An **Add New Particles** dialog box appears. Assign the numbers of particles to the edit fields in the dialog box as shown in Fig. 2.16. Click the **Properties** tab and click the colored button to select an appropriate color for the new particles. When finished, click **OK**.

f. To set particles around the pumping well in the second and third layer, press PgDn to move down a layer and repeat steps c, d and e. Use other colors for the new particles in the second and third layers.

g. Click  to start the backward particle tracking.
PMPATH calculates and shows the projections of the pathlines as well as the capture zone of the pumping well (Fig. 2.17).

To see the projection of the pathlines on the cross-section windows in greater details, open an **Environment Options** dialog box by choosing **Environment...** from the **Options** menu and set a larger **exaggeration** value for the vertical scale in the **Cross Sections** tab. Fig. 2.18 shows the same pathlines by setting the vertical exaggeration value to 10. Note that some pathlines end up at the groundwater surface, where recharge occurs. This is one of the major differences between a three-dimensional and a two-dimensional model. In two-dimensional areal simulation models, such as ASM for Windows (Chiang et al., 1998), FINEM (Kinzelbach et al, 1990) or MOC (Konikow and Bredehoeft, 1978), a vertical velocity term does not exist (or always equals to zero). This leads to the result that pathlines can never be tracked back to the ground surface where the groundwater recharge from the precipitation occurs.

PMPATH can create time-related capture zones of pumping wells. The 100-days-capture zone shown in Fig. 2.19 is created by using the settings in the **Particle Tracking (Time) Properties** dialog box (Fig. 2.20) and clicking  . To open this dialog box, choose **Particle Tracking (Time)...** from the **Options** menu. Note that because of lower hydraulic conductivity (and thus lower flow velocity) the capture zone in the first layer is smaller than those in the other layers.

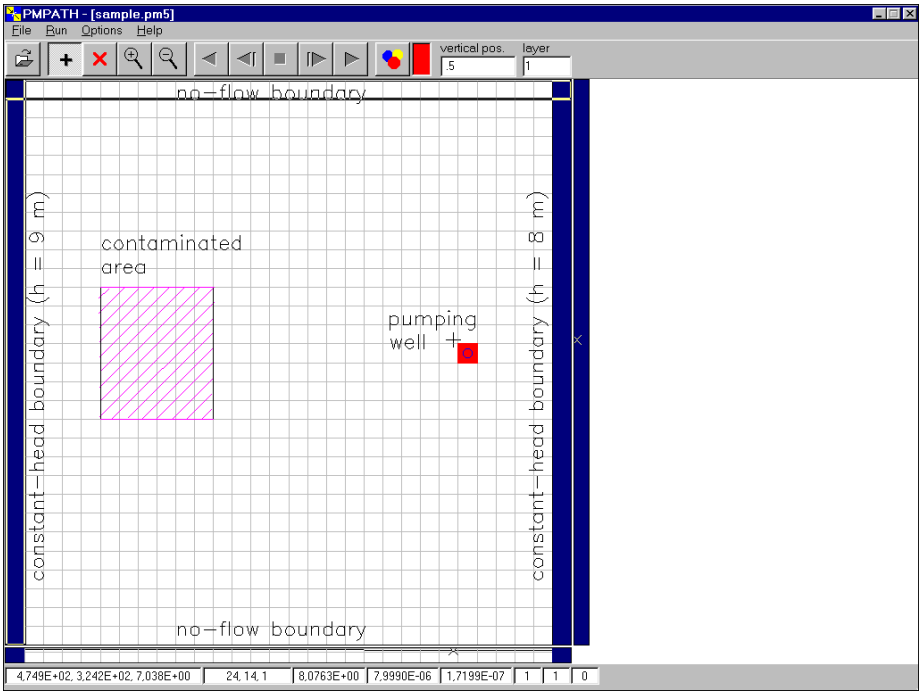


Fig. 2.15 The sample model loaded in PMPATH

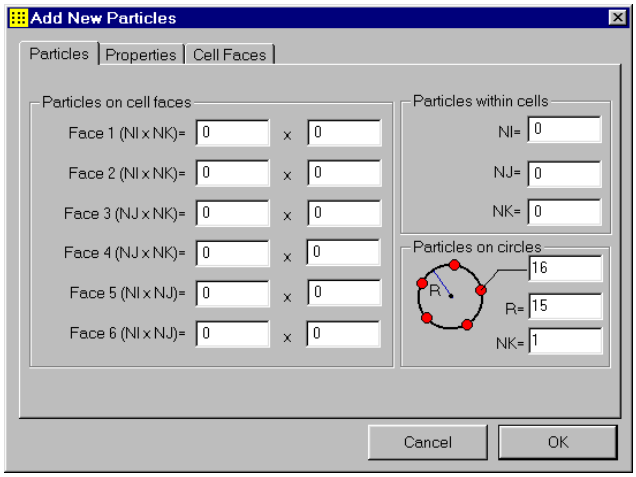


Fig. 2.16 The **Add New Particles** dialog box

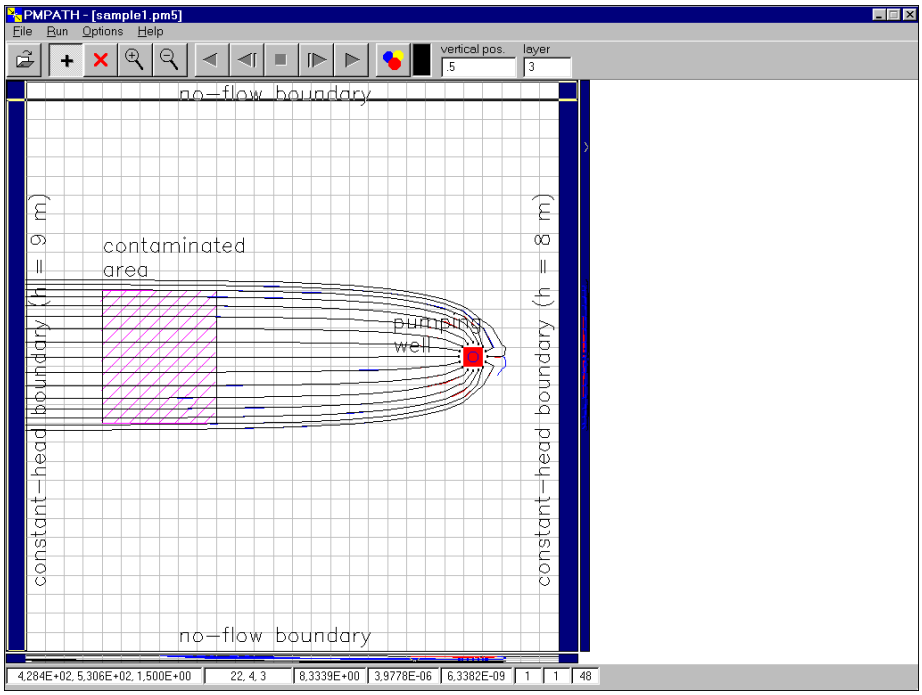


Fig. 2.17 The capture zone of the pumping well (with vertical exaggeration=1)

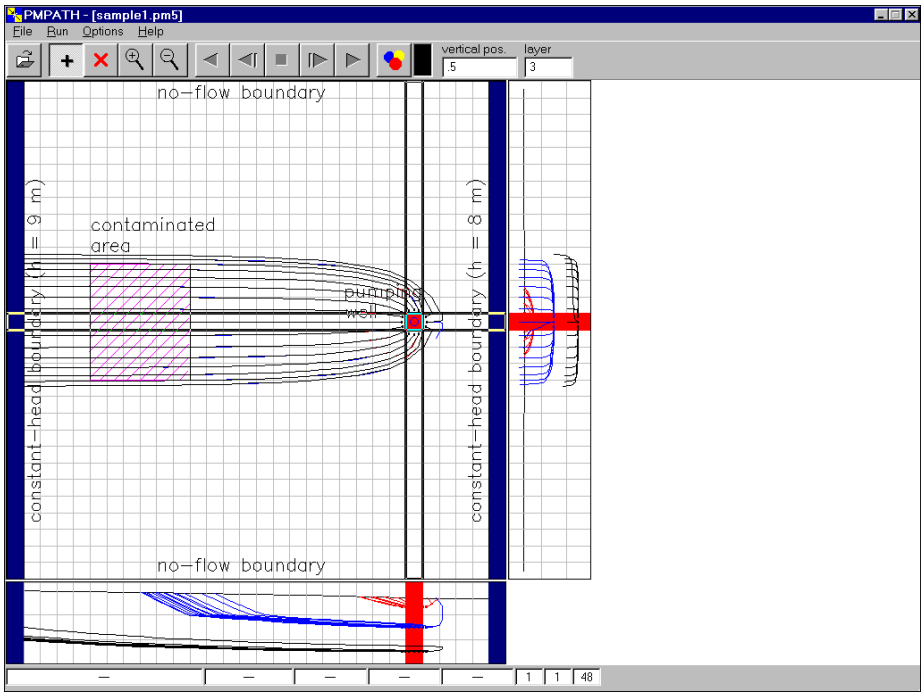


Fig. 2.18 The capture zone of the pumping well (with vertical exaggeration=10)

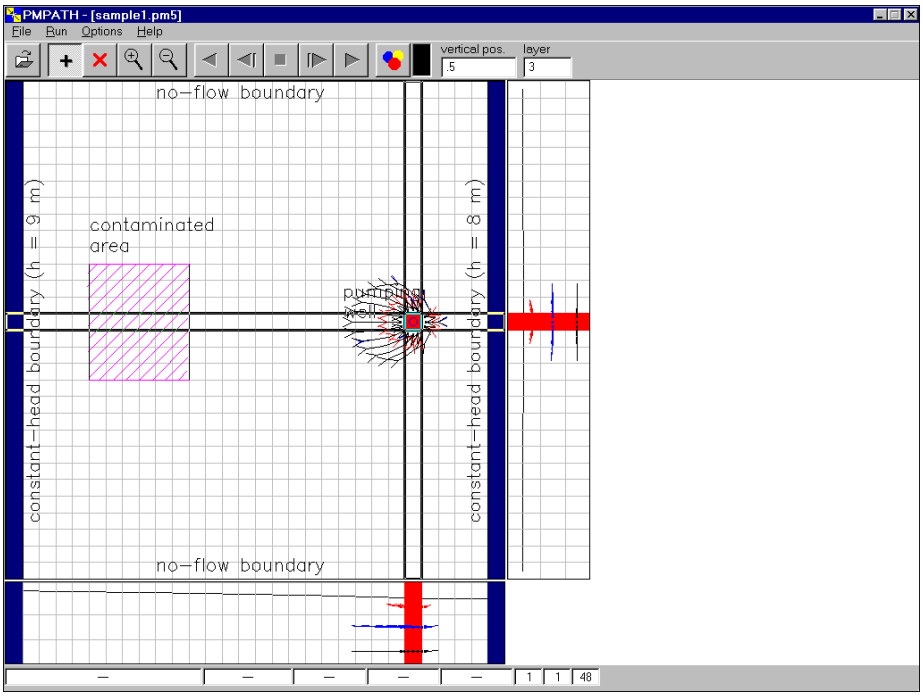


Fig. 2.19 100-days-capture zone calculated by PMPATH

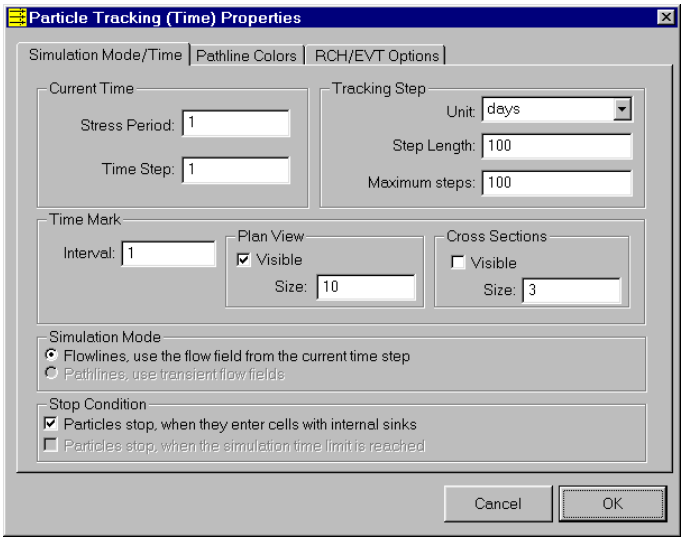


Fig. 2.20 The **Particle Tracking (Time) Properties** dialog box

2.2 Simulation of Solute Transport

Basically, the transport of solutes in porous media can be described by three processes: *advection*, *hydrodynamic dispersion* and *physical, chemical or biochemical reactions*.

Both the MT3D and MOC3D models use the *method-of-characteristics* (MOC) to simulate the advection transport, in which dissolved chemicals are represented by a number of particles and the particles are moving with the flowing groundwater. Besides the MOC method, the MT3D and MT3DMS models provide other methods for solving the advective term, see sections 3.6.3 and 3.6.4 for details.

The hydrodynamic dispersion can be expressed in terms of the *dispersivity* [L] and the *coefficient of molecular diffusion* [L^2T^{-1}] for the solute in the porous medium. The types of reactions incorporated into MOC3D are restricted to those that can be represented by a first-order rate reaction, such as radioactive decay, or by a retardation factor, such as instaneous, reversible, sorption-desorption reactions goverened by a linear isotherm and constant distribution coefficient (K_d). In addition to the linear isotherm, MT3D supports non-linear isotherms, i.e., Freundlich and Langmuir isotherms.

Prior to running MT3D or MOC3D, you need to define the observation boreholes, for which the breakthrough curvers will be calculated.

▸ **To define observation boreholes**

1. Choose **Boreholes and Observations** from the **Paramters** menu.

   A **Boreholes and Observations** dialog box appears. Enter the coordinates of the observation boreholes into the dialog box as shown in Fig. 2.21.
2. Click **OK** to close the dialog box.

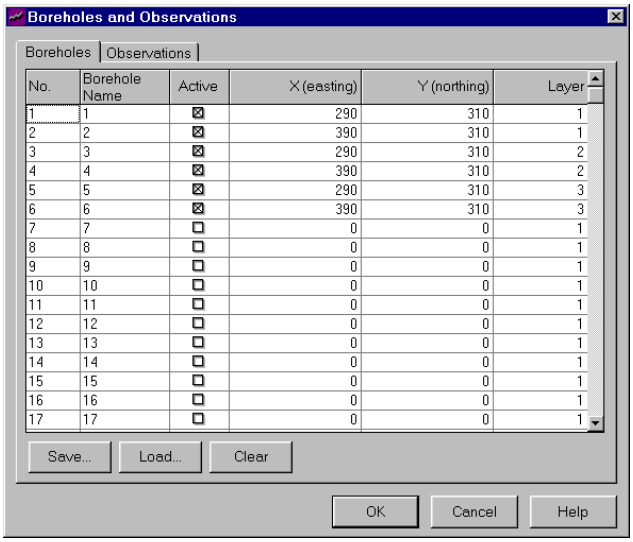


Fig. 2.21 The **Boreholes and Observations** dialog box

2.2.1 Perform Transport Simulation with MT3D

MT3D requires a boundary condition code for each model cell which indicates whether (1) solute concentration varies with time (active concentration cell), (2) the concentration is kept fixed at a constant value (constant-concentration cell), or (3) the cell is an inactive concentration cell. Use 1 for an active concentration cell, -1 for a constant-concentration cell, and 0 for an inactive concentration cell. Active, variable-head cells can be treated as inactive concentration cells to minimize the area needed for transport simulation, as long as the solute concentration is insignificant near those cells.

Similar to the flow model, you must specify the initial concentration for each model cell. The initial concentration at a constant-concentration cell will be kept constant during a transport simulation. The other concentration are starting values in a transport simulation.

▸ **To assign the boundary condition to MT3D**

1. Choose **Boundary Conditions ▸ ICBUND (MT3D/MT3DMS)** from the **Grid** menu.
   For the current example, we accept the default value 1 for all cells.
2. Choose **Leave Editor** from the **File** menu or click the **leave editor** button  .

▸ **To set the initial concentration**

1. Choose **MT3D ▸ Initial Concentration** from the **Models** menu.
   For the current example, we accept the default value 0 for all cells.
2. Choose **Leave Editor** from the **File** menu or click the **leave editor** button  .

▸ **To assign the input rate of contaminants**

1. Choose **MT3D ▸ Sink/Source Concentration ▸ Recharge** from the **Models** menu.
2. Assign 12500 [µg/m^3] to the cells within the contaminated area.
   This value is the concentration associated with the recharge flux. Since the recharge rate is 8×10^{-9} [$m^3/m^2/s$] and the dissolution rate is 1×10^{-4} [µg/s/m^2], the concentration associated with the recharge flux is $1 \times 10^{-4} / 8 \times 10^{-9} = 12500$ [µg/m^3]
3. Choose **Leave Editor** from the **File** menu or click the **leave editor** button  .

▸ **To assign the transport parameters to the Advection Package**

1. Choose **MT3D ▸ Advection...** from the **Models** menu.
   An **Advection Package (MTADV1)** dialog box appears. Enter the values as shown in Fig. 2.22 into the dialog box, select **Method of Characteristics (MOC)** for the solution scheme and **First-order Euler** for the particle tracking algorithm.

2. Click **OK** to close the dialog box.

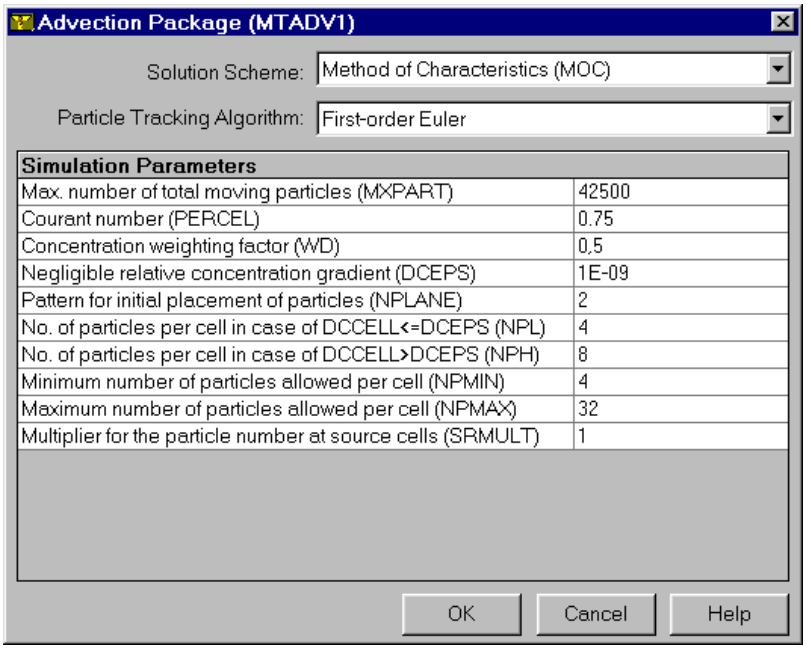


Fig. 2.22 The **Advection Package (MTADV1)** dialog box

▸ **To assign the dispersion parameters**

1. Choose **MT3D ▸ Dispersion...** from the **Models** menu.
   A **Dispersion Package (MT3D)** dialog box appears. Enter the ratios of the transverse dispersivity to longitudinal dispersivity as shown in Fig. 2.23.
2. Click **OK**.
   PMWIN displays the model grid. At this point you need to specify the longitudinal dispersivity to each cell of the grid.
3. Choose **Reset Matrix...** from the **Value** menu (or press Ctrl+R), type 10 in the dialog box then click **OK**.
4. Turn on **layer copy** by clicking the **layer copy** button .
5. Move to the second layer and the third layer by pressing PgDn twice.
   The cell values of the first layer are copied to the second and third layers.
6. Choose **Leave Editor** from the **File** menu or click the **leave editor** button .

▸ **To assign the chemical reaction parameters**

1. Choose **MT3D ▸ Chemical Reaction ▸ Layer by Layer** from the **Models** menu.
   A **Chemical Reaction Package (MTRCT1)** dialog box appears. Clear the check box **Simulate the radioactive decay or biodegradation** and select **Linear equlibrium**

isotherm for the type of sorption. For the linear isotherm, the retardation factor **R** for each cell is calculated at the beginning of the simulation by

$$R = 1 + \frac{\rho_b}{n} \cdot K_d \qquad (2.3)$$

Where n [-] is the effective porosity with respect to the flow through the porous medium, ρ_b [ML^{-3}] is the bulk density of the porous medium and K_d [L^3M^{-1}] is the distribution coefficient of the solute in the porous medium. As the effective porosity is equal to 0.25, setting ρ_b = 2000 and K_d = 0.000125 yields R = 2.

2. Click **OK** to close the **Chemical Reaction Package (MTRCT1)** dialog box (Fig. 2.24).

The last step before running the transport model is to specify the output times, at which the calculated concentration should be saved.

▸ **To specify the output times**

1. Choose **MT3D ▸ Output Control...** from the **Models** menu.
   An **Output Control (MT3D, MT3DMS)** dialog box appears. The options in this dialog box are grouped under three tabs - **Output Terms**, **Output Times** and **Misc**.
2. Click the **Output Times** tab, then click the header **Output Time** of the (empty) table.
   An **Output Times** dialog box appears. Enter 3000000 to **Interval** in this dialog box then click **OK** to accept the other defalut values.
3. Click **OK** to close the **Output Control (MT3D, MT3DMS)** dialog box (Fig. 2.25).

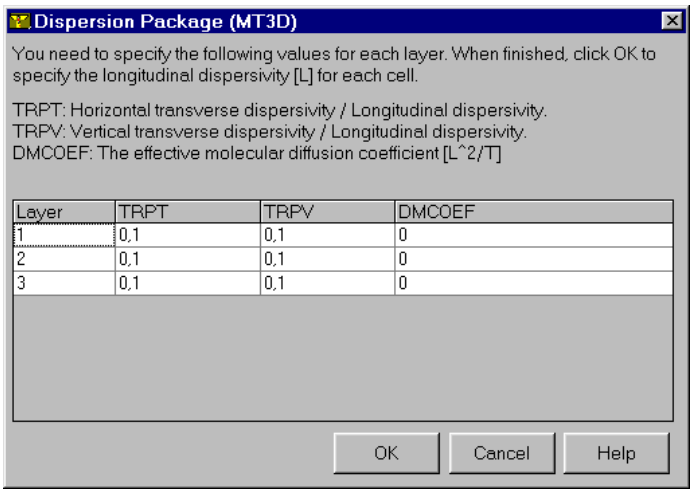


Fig. 2.23 The **Advection Package (MTADV1)** dialog box

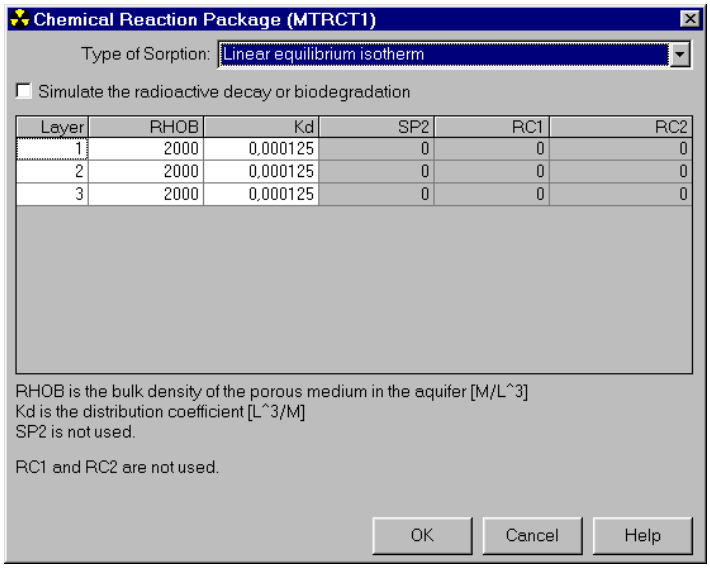


Fig. 2.24 The **Chemical Reaction Package (MTRCT1)** dialog box

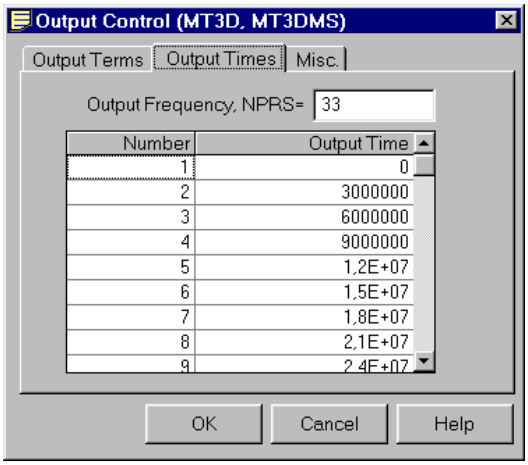


Fig. 2.25 The **Output Control (MT3D, MT3DMS)** dialog box

- **To perform the transport simulation**

1. Choose **MT3D▸Run...** from the **Models** menu.
   The **Run MT3D/MT3D96** dialog box appears (Fig. 2.26).
2. Click **OK** to start the transport computation.
   Prior to running MT3D, PMWIN will use user-specified data to generate input files for MT3D as listed in the table of the **Run MT3D/MT3D96** dialog box. An input file will be generated, only if the **generate** flag is set to ☒. You can click on the button to toggle the **generate** flag between ☒ and ☐. Generally, you do not need to change the flags, as PMWIN will care about the settings.

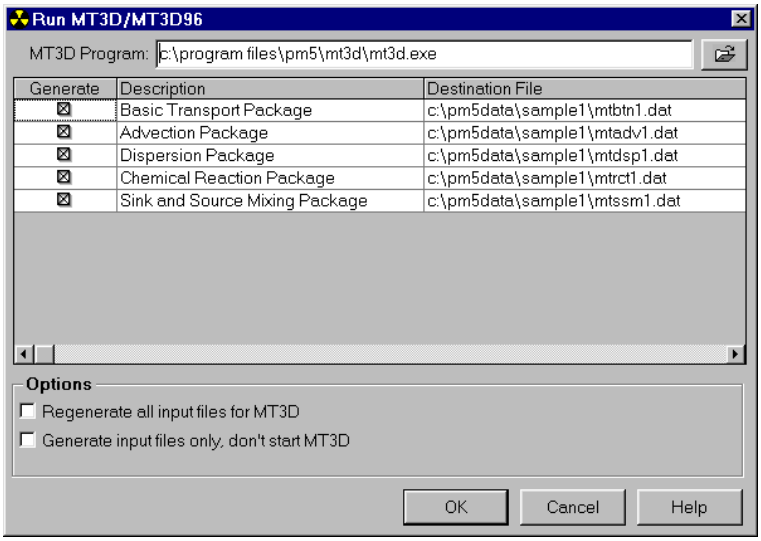


Fig. 2.26 The **Run MT3D/MT3D96** dialog box

- **Check simulation results and produce output**

During a transport simulation, MT3D writes a detailed run record to the file *path*\OUTPUT.MT3, where *path* is the folder in which your model data are saved. MT3D saves the simulation results in various files, which can be controlled by choosing **MT3D ▸ Output Control...** from the **Models** menu.

To check the quality of the simulation results, a mass budget is calculated at the end of each transport step and accumulated to provide summarized information on the total mass into or out of the groundwater flow system. The discrepancy between the total mass in and out servers as an indicator of the accuracy of the simulation results. It is highly recommended to check the record file or at least take a glance at it.

Using **Presentation** you can generate contour maps of the calculated concentration. Fig. 2.27 shows the calculated concentration in the third layer at the end of the simulation (simulation time=9.467E+07 seconds).

To generate the breakthrough curves, choose **Graphs ▸ Concentration Time ▸ MT3D** from the **Tools** menu. Click on the **Plot** flags of the **Boreholes** table until they are set to ☒ (Fig. 2.28).

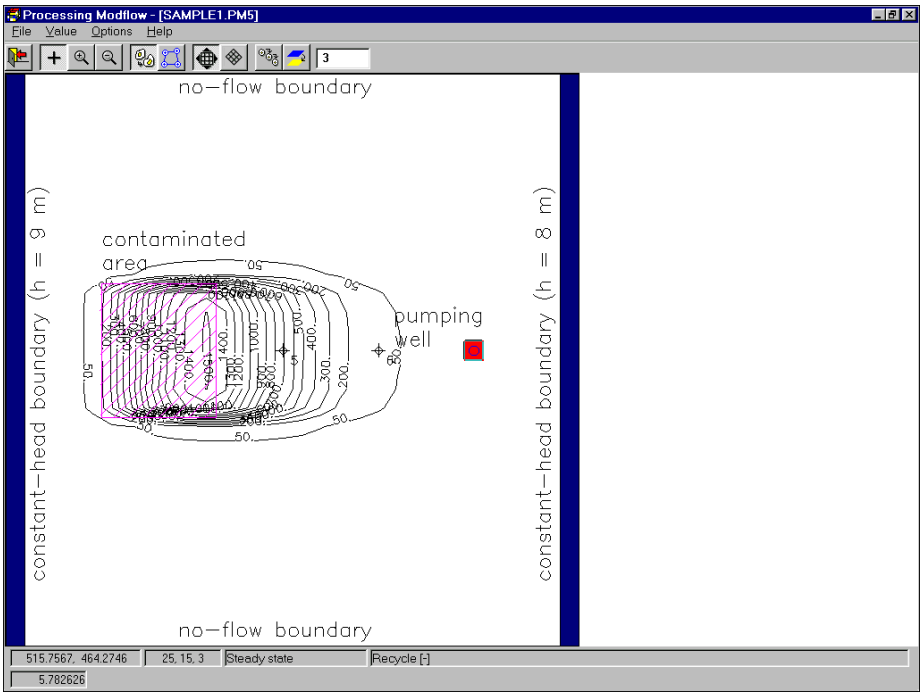


Fig. 2.27 Simulated concentration at 3 years in the third layer

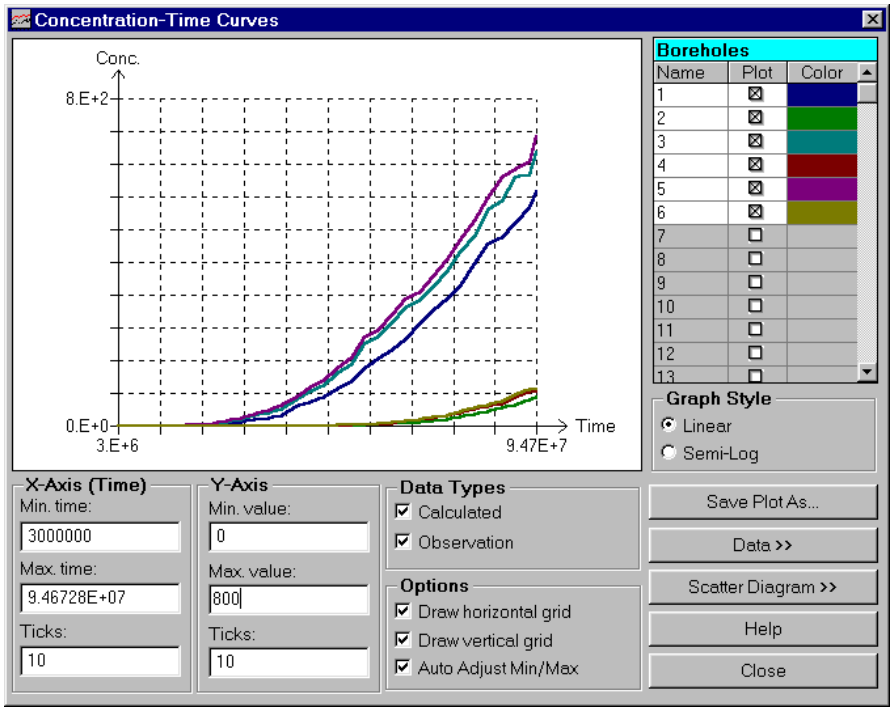


Fig. 2.28 Concentration-time curves at the observation boreholes

2.2.2 Perform Transport Simulation with MOC3D

In MOC3D, transport may be simulated within a subgrid, which is a "window" within the primary model grid used to simulate flow. Within the subgrid, the row and column spacing must be uniform, but the thickness can vary from cell to cell and layer to layer. However, the range in thickness values (or product of thickness and effective porosity) should be as small as possible.

The initial concentration must be specified throughout the subgrid within which solute transport occurs. MOC3D assumes that the concentration outside of the subgrid is the same within each layer, so only one value is specified for each layer within and adjacent to the subgrid. The use of constant-concentration boundary condition has not been implemented in MOC3D.

▸ **To set the initial concentration**

1. Choose **MOC3D ▸ Initial Concentration** from the **Models** menu.
   For the current example, we accept the default value 0 for all cells. Note that PMWIN automatically uses the same initial concentration values for both MOC3D and MT3D.
2. Choose **Leave Editor** from the **File** menu or click the **leave editor** button  .

▸ **To define the transport subgrid and the concentration outside of the subgrid**

1. Choose **MOC3D ▸ Subgrid...** from the **Models** menu.
   The **Subgrid for Transport (MOC3D)** dialog box appears (Fig. 2.29). The options in the dialog box are grouped under two tabs - **Subgrid** and **C' Outside of Subgrid**. The default size of the subgrid is the same as the model grid used to simulate flow. The default initial concentration outside of the subgrid is zero. We will accept the defaults.
2. Click **OK** to accept the default values and close the dialog box.

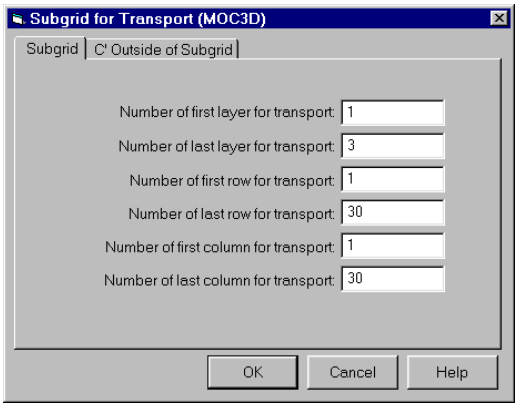


Fig. 2.29 The **Subgrid for Transport (MOC3D)** dialog box.

▸ **To assign the input rate of contaminants**

1. Choose **MOC3D ▸ Sink/Source Concentration ▸ Recharge** from the **Models** menu.
2. Assign 12500 [µg/m^3] to the cells within the contaminated area.
   This value is the concentration associated with the recharge flux. Since the recharge rate is 8×10^{-9} [$m^3/m^2/s$] and the dissolution rate is 1×10^{-4} [µg/s/m^2], the concentration associated with the recharge flux is $1 \times 10^{-4} / 8 \times 10^{-9} = 12500$ [µg/m^3]
3. Choose **Leave Editor** from the **File** menu or click the **leave editor** button  .

▸ **To assign the parameters for the advective transport**

1. Choose **MOC3D ▸ Advection...** from the **Models** menu.
   A **Parameters for Advection Transport (MOC3D)** dialog box appears. Enter the values as shown in Fig. 2.30 into the dialog box, select **Bilinear (X, Y directions)** for the interpolation scheme for particle velocity. As noted by Konikow et al. (1996), if transmissivity within a layer is homogeneous or smoothly varying, bilinear interpolation of velocity yields more realistic pathlines for a given discretization than does linear interpolation.
2. Click **OK** to close the dialog box.

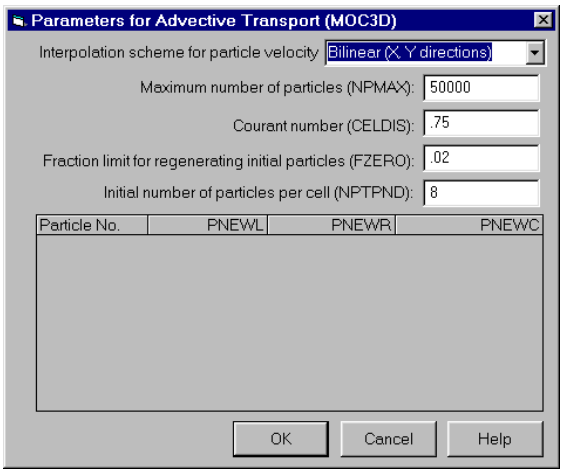


Fig. 2.30 The **Parameters for Advective Transport** dialog box.

▸ **To assign the parameters for dispersion and chemical reaction**

1. Choose **MOC3D ▸ Dispersion & Chemical Reaction...** from the **Models** menu.
   A **Dispersion / Chemical Reaction (MOC3D)** dialog box appears. Check **Simulate Dispersion** and enter the values as shown in Fig. 2.31. Note that the parameters for dispersion and chemical reaction are the same for each layer.
2. Click **OK** to close the dialog box.

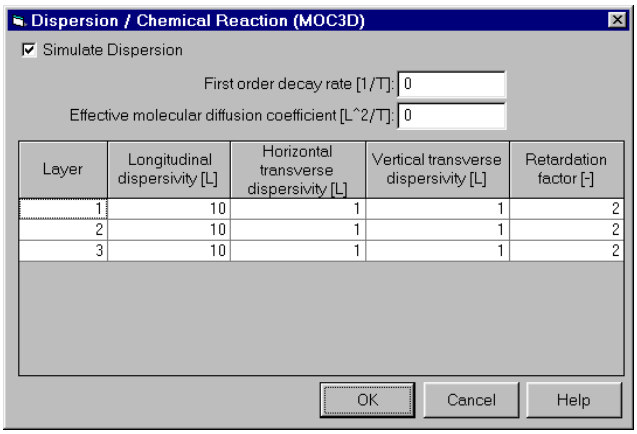


Fig. 2.31 The **Dispersion / Chemical Reaction (MOC3D)** dialog box.

▸ **To set Strong/Weak Flag**

1. Choose **MOC3D ▸ Strong/Weak Flag** from the **Models** menu.
2. Move the grid cursor to the cell [25, 15, 1].
3. Press the right mouse button and type 1, then click OK. Note that a strong sink or source is indicated by the value of 1 in the matrix. When a fluid source is "strong", new particles are added to replace old particles as they are advected out of that cell. Where a fluid sink is "strong", particles are removed after they enter that cell.
4. Repeat steps 2 and 3 to assign the value 1 to the cells [25, 15, 2] and [25, 15, 3].
5. Choose **Leave Editor** from the **File** menu or click the **leave editor** button .

▸ **To specify the output terms and times**

1. Choose **MOC3D ▸ Output Control...** from the **Models** menu.
   An **Output Control (MOC3D)** dialog box appears. The options in the dialog box are grouped under five tabs - **Concentration**, **Velocity**, **Particle Locations**, **Disp. Coeff.** and **Misc**.
2. In the **Concentration** tab, select the option **These data will be printed or saved every Nth particle moves** and enter **N** = 20.
3. Click **OK** to accept all other default values and close the **Output Control (MOC3D)** dialog box (Fig. 2.32).

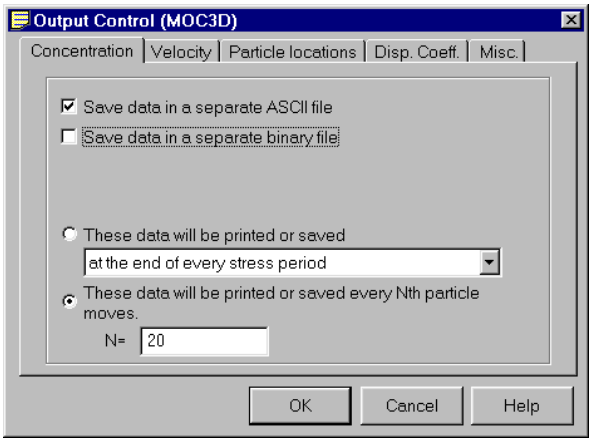


Fig. 2.32 The **Output Control (MOC3D)** dialog box.

- **To perform the transport simulation**

1. Choose **MOC3D▸Run...** from the **Models** menu.
   The **Run MOC3D** dialog box appears (Fig. 2.33).
2. Click **OK** to start the transport computation.
   Prior to running MOC3D, PMWIN will use user-specified data to generate input files for MOC3D as listed in the table of the **Run MOC3D** dialog box. An input file will be generated, only if the **generate** flag is set to ☒. You can click on the button to toggle the **generate** flag between ☒ and ☐. Generally, you do not need to change the flags, as PMWIN will care about the settings.

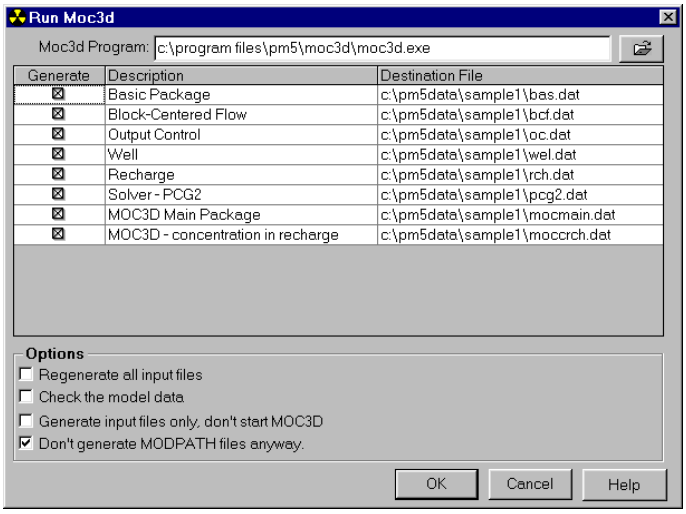


Fig. 2.33 The **Run MOC3D** dialog box

▸ **Check simulation results and produce output**

During a transport simulation, MOC3D writes a detailed run record to the file *path*\MOC3D.LST, where *path* is the folder in which your model data are saved. MOC3D saves the simulation results in various files, which can be controlled by choosing **MOC3D ▸ Output Control...** from the **Models** menu.

To check the quality of the simulation results, mass balance calculations are performed and saved in the run record file. The mass in storage at any time is calculated from the concentrations at the nodes of the transport subgrid to provide summarized information on the total mass into or out of the groundwater flow system. The mass balance error will typically exhibit an oscillatory behavior over time, because of the finite-difference approximation and the nature of the method of characteristics. As discussed in Konikow et al. (1996), as long as the oscillations remain within a steady range, not exceeding about ±10 percent as a guide, then the error probably does not represent a bias and is not a serious problem. Rather, the ocillations only reflect the fact that **the mass balance calculation is itself just an approximation**.

Using **Presentation** you can generate contour maps of the calculated concentration. Fig. 2.34 shows the calculated concentration at 3 years in the third layer (simulation time=9.467E+07 seconds).

To generate the breakthrough curves, choose **Graphs ▸ Concentration Time ▸ MOC3D** from the **Tools** menu. Click on the **Plot** flags of the **Boreholes** table until they are set as in Fig. 2.35.

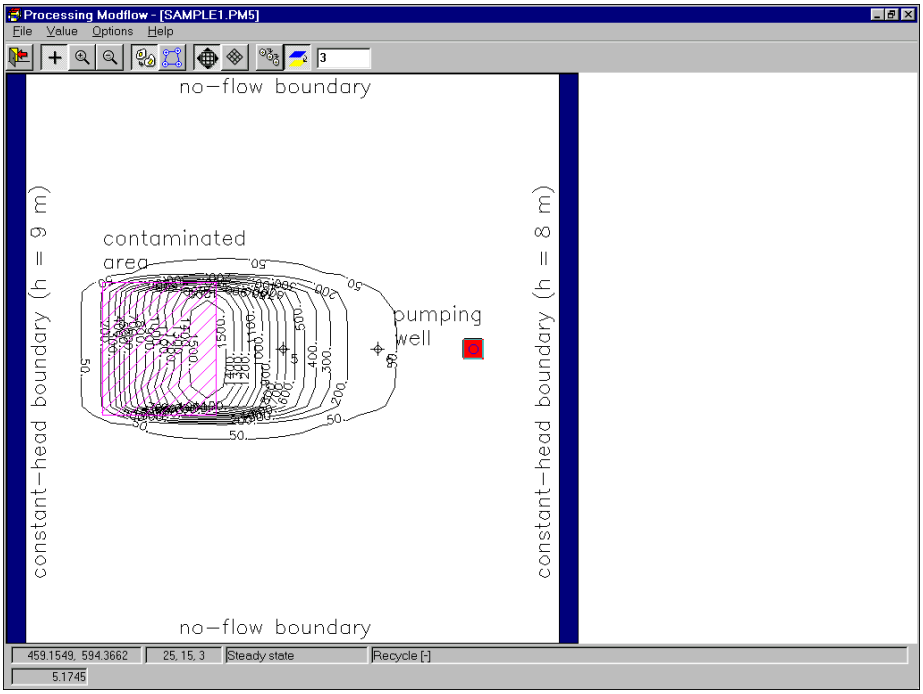


Fig. 2.34 Simulated concentration at 3 years in the third layer

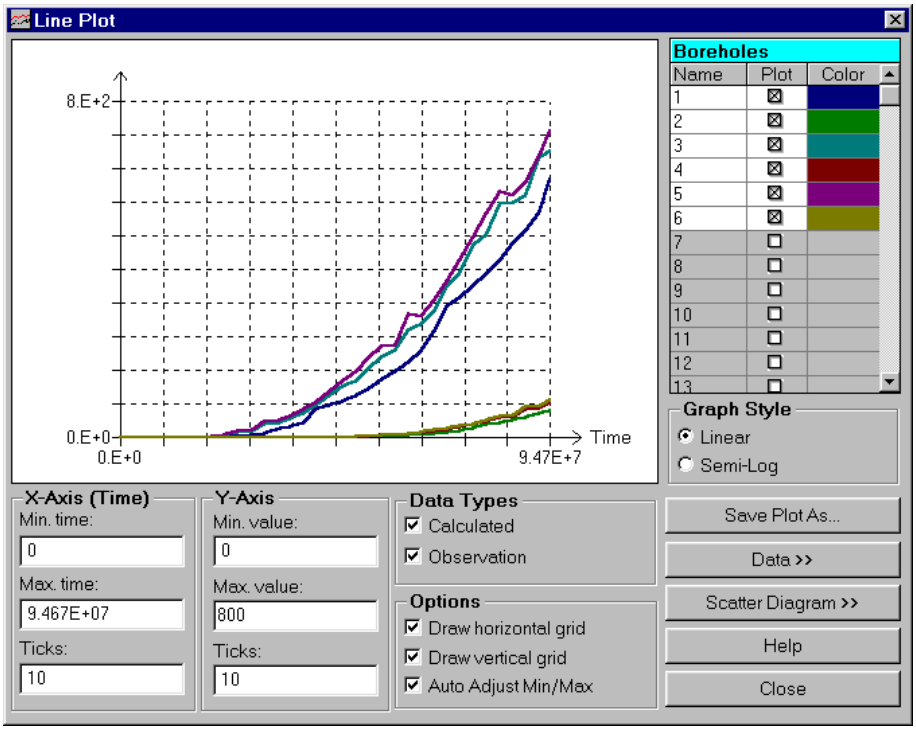


Fig. 2.35 Concentration-time curves at the observation boreholes

2.3 Automatic Calibration

Calibration of a flow model is accomplished by finding a set of parameters, hydrologic stresses or boundary conditions so that the simulated heads or drawdowns match the measurement values to a reasonable degree. The calibration process is one of the most difficult and critical steps in the model application. Hill (1998) gives methods and guidelines for model calibration using inverse modeling.

To demonstrate the use of the inverse models PEST and UCODE within PMWIN, we assume that the hydraulic conductivity in the third layer is homogeneous but its value is unknown. We want to find out this value through a model calibration by using the measured hydraulic heads at the observation boreholes listed below.

Borehole	X-coordinate	Y-coordinate	Layer	Hydraulic Head
1	130	200	3	8.85
2	200	400	3	8.74
3	480	250	3	8.18
4	460	450	3	8.26

Three steps are required for an automatic calibration.

1. Assign the zonal structure of each parameter.
   Automatic calibration requires a subdivision of the model domain into a small number of reasonable zones of equal parameter values. The zonal structure is given by assigning to each zone a parameter number in the **Data Editor**.
2. Specify the coordinates of the observation boreholes and the measured hydraulic heads.
3. Specify the starting values, upper and lower bounds for each parameter.

▸ **To assign the zonal structure to the horizontal hydraulic conductivity**

1. Choose **Horizontal Hydraulic Conductivity** from the **Parameters** menu.
2. Move to the third layer by pressing PgDn twice.
3. Choose **Reset Matrix...** from the **Value** menu (or press Ctrl+R).
   A **Reset Matrix** dialog box appears.
4. Enter 1 to the **Parameter Number** edit box, then click **OK**.
   The horizontal hydraulic conductivity of the third layer is set to the parameter #1.
5. Choose **Leave Editor** from the **File** menu or click the **leave editor** button  .

Note that for layers of type **0:confined** and **2:confined/unconfined (transmissivity=const.)**, MODFLOW reads transmissvity (instead of hydraulic conductivity) from the model data file, consequently we are actually calibrating the transmissivity and must use suitable values for the initial guess and lower and upper bounds. Change the layer type to **3:confined/unconfined (transmissivity varies)**, if you want to calibrate the horizontal hydraulic conductivity.

▸ **To specify the coordinates of the observation boreholes and measured values**

1. Choose **Boreholes and Observations** from the **Parameters** menu and enter the coordinates of the observation boreholes into the boreholes table.
2. Click the **Observations** tab and enter the values into the observations table as shown in Fig. 2.36. Note that the observation time, to which the measurement pertains, is measured from the beginning of the model simulation. For a steady state simulation with one stress period (you can run a steady state simulation over several stress periods), the length of the period (9.46728E+07 seconds) is given as the observation time.
3. Click **OK** to close the dialog box.

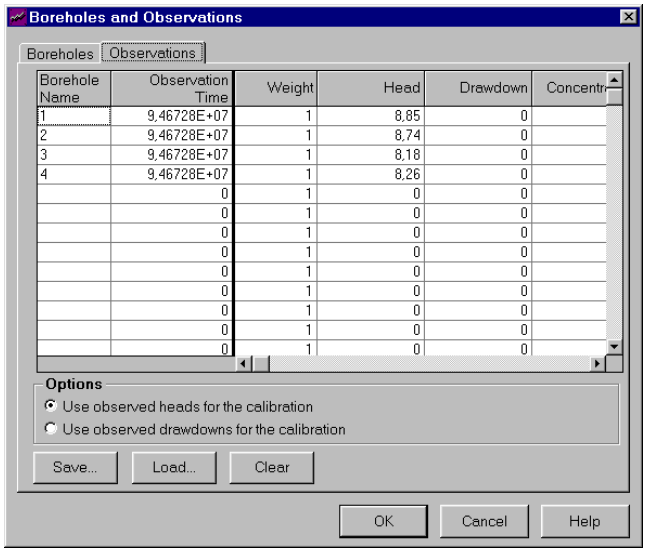


Fig. 2.36 The **Boreholes and Observations** dialog box

2.3.1 Perform Automatic Calibration with PEST

▸ **To specify the starting values for each parameter**

1. Choose **PEST ▸ Parameter List...** from the **Models** menu.
   A **List of Calibration Parameters (PEST)** dialog box appears. The options of the dialog box are grouped under five tabs - **Parameters**, **Group Definitions**, **Prior Information**, **Control Data** and **Options**.
2. In the **Parameters** tab, activate the first parameter (by setting the Active flag to ☒) from Parameters table and enter values shown in Fig. 2.37 into the table. **PARVAL1** is the initial guess of the parameter. **PARLBUD** is the lower bound and **PARUBUD** is the upper bound of the parameter.

▸ **To perform the automatic calibration**

1. Choose **PEST (Inverse Modeling) ▸ Run...** from the **Models** menu.
   The **Run PEST** dialog box appears (Fig. 2.38).
2. Click **OK** to start the calibration.
   Prior to running PEST, PMWIN will use user-specified data to generate input files for PEST and MODFLOW as listed in the table of the **Run PEST** dialog box. An input file will be generated, only if the **generate** flag is set to ☒. You can click on the button to toggle the **generate** flag between ☒ and ☐. Generally, you do not need to change the flags, as PMWIN will care about the settings.

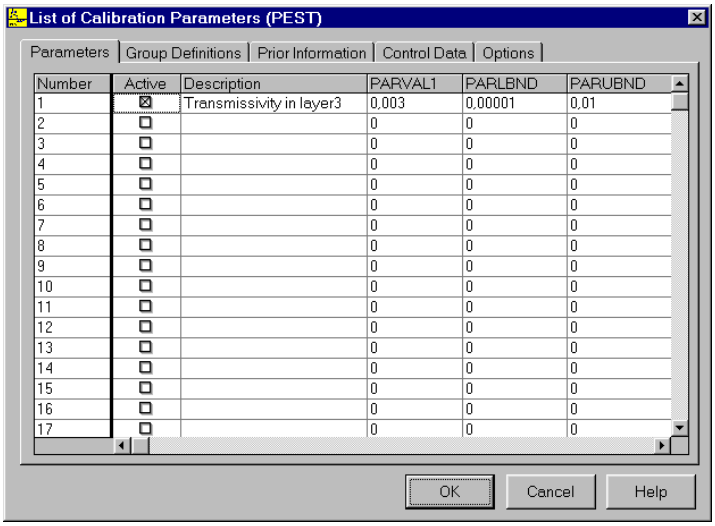


Fig. 2.37 The **List of Calibration Parameters (PEST)** dialog box

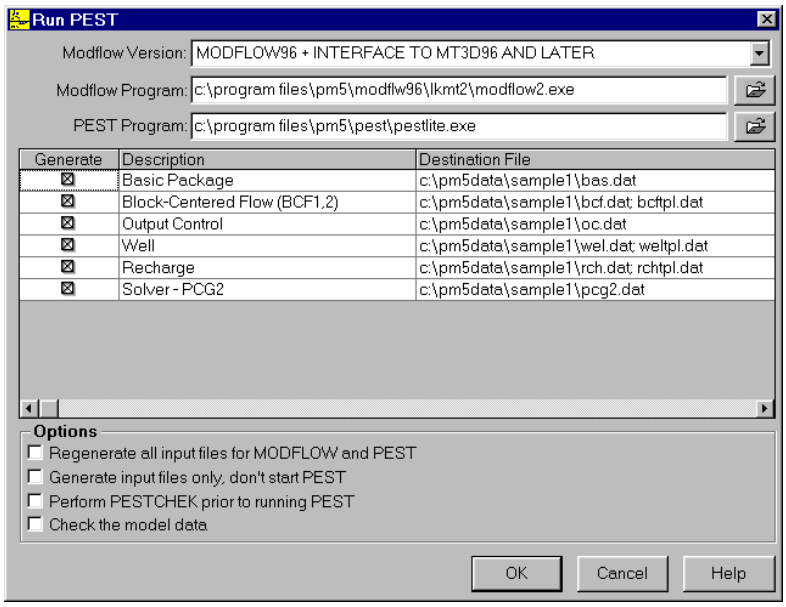


Fig. 2.38 The **Run PEST** dialog box

Check calibration results

During the automatic calibration several result files are created. PEST writes the optimized parameter values to the input files of MODFLOW (BCF.DAT, WEL.DAT, etc.) and creates a detailed run record file *path*\PESTCTL.REC, where *path* is the folder in which your model data are saved. The simulation results of MODFLOW are updated by using the optimized parameter values, which are saved in a separate file PESTCTL.PAR.

Note that PMWIN does not retrieve the optimized parameter values into the data matrices. Your (PMWIN-) model data will not be modified in any way. This provides more security for the model data, because an automatic calibration process does not necessarily lead to a success. If you want to operate on a calibrated model, you can **import** the model by choosing **Convert Model...** from the **File** menu, see Chapter 3 for details.

You can create a scatter diagram to present the calibration result. The observed head values are plotted on one axis against the corresponding calculated values on the other. If there is exact agreement between measurement and simulation, all points lie on a 45° line. The narrower the area of scatter around this line, the better is the match.

▸ **To create a scatter diagram for head values**

1. Choose **Graph ▸ Head-Time** from the **Tools** menu.
   A **Head-Time Curves** dialog box appears.
2. Click the button **Scatter Diagram »**
   PMWIN shows the scatter diagram (Fig. 2.39). See Chapter 5 for details about the use of this dialog box.

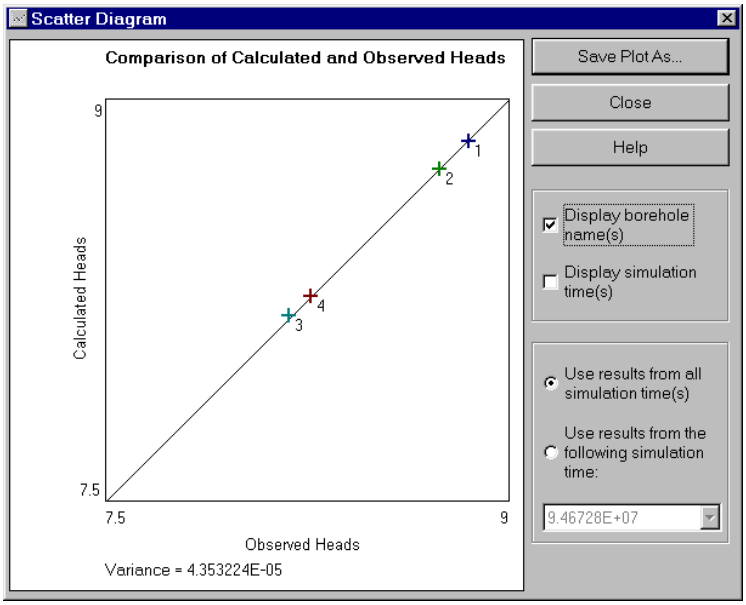


Fig. 2.39 The **Scatter Diagram** dialog box

2.3.2 Perform Automatic Calibration with UCODE

▸ **To specify the starting values for each parameter**

1. Choose **UCODE ▸ Parameter List...** from the **Models** menu.
   A **List of Calibration Parameters (UCODE)** dialog box appears. The options of the dialog box are grouped under five tabs - **Parameters**, **Prior Information**, **Control Data** and **Options**.
2. In the **Parameters** tab, activate the first parameter (by setting the Active flag to ☒) from Parameters table and enter values shown in Fig. 2.40 into the table. **Start-value** is the initial guess of the parameter. **Minimum** is the reasonable minimum value and **Maximum** is the reasonable maximum value for the parameter. These two values are used solely to determine how the final optimized value of the parameter compares to a reasonable range of values.
3. Check the **Log-transform** flag to log-transform the parameter. This will ensure that only positive values will be used for the parameter during the calibration.

▸ **To perform the automatic calibration**

1. Choose **UCODE (Inverse Modeling) ▸ Run...** from the **Models** menu.
   The **Run UCODE** dialog box appears (Fig. 2.41).
2. Click **OK** to start the calibration.
   Prior to running UCODE, PMWIN will use user-specified data to generate input files for UCODE and MODFLOW as listed in the table of the **Run UCODE** dialog box. An input file will be generated, only if the **generate** flag is set to ☒. You can click on the button to toggle the **generate** flag between ☒ and ☐. Generally, you do not need to change the flags, as PMWIN will care about the settings.

Check calibration results

During the automatic calibration several result files are created. Similar to PEST, UCODE writes the optimized parameter values to the input files of MODFLOW (BCF.DAT, WEL.DAT, etc.) and creates a detailed run record file *path*\ucode._ot, where *path* is the folder in which your model data are saved. The simulation results of MODFLOW are updated by using the optimized parameter values, which are saved in a separate file ucode._st. Similar to PEST, you can create a scatter diagram to present the calibration result (see above).

Note that PMWIN does not retrieve the optimized parameter values into the data matrices. Your (PMWIN-) model data will not be modified in any way. This provides more security for the model data, because an automatic calibration process does not necessarily lead to a success. If

you want to operate on a calibrated model, you can **import** the model by choosing **Convert Model...** from the **File** menu, see Chapter 3 for details.

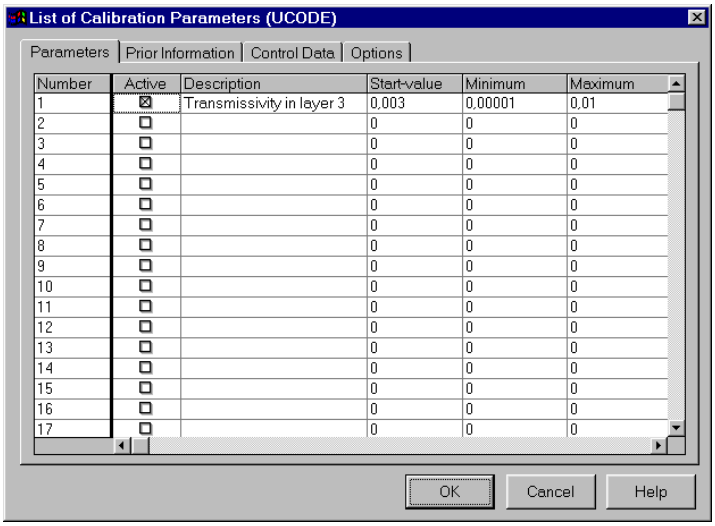


Fig. 2.40 The **List of Calibration Parameters (UCODE)** dialog box

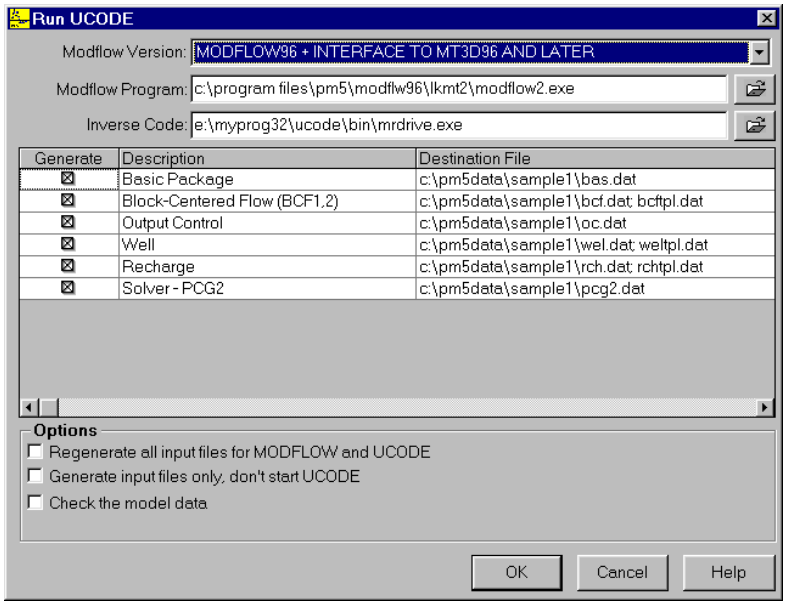


Fig. 2.41 The **Run UCODE** dialog box

2.4 Animation

You already learned how to use the **Presentation** tool to create and print contour maps from calculated head and concentration values. The saved or printed images are static and ideal for paper-reports. In many cases, however, these static images cannot ideally illustrate motion of concentration plumes or temporal variation of hydraulic heads or drawdowns. PMWIN provides an animation technique to display a sequence of the saved images in rapid succession. Although the animation process requires relatively large amount of computer resources to read, process and display the data, the effect of a motion picture is often very helpful.

The **Presentation** tool is used to create animation sequences. The following steps show how to use the **Environment Options** and **Animation** dialog boxes to create an animation sequence for displaying the motion of the concentration plume in the third layer.

- **To create an animation sequence**

1. Choose **Presentation** from the **Tools** menu.
2. Move to the third layer by pressing **PgDn** twice.
3. Choose **Environment...** from the **Options** menu
4. Click the **Contours** tab, clear **Display contour lines,** and check **Visible** and **Fill Colors**.
5. Click the table header **Level**.
   A **Contour Levels** dialog box appears. Set **Minimum** to 100, **Maximum** to 1600 and **Interval** to 100. These values are used, because we already know the range of the concentration values from Fig. 2.27. When finished, click **OK** to close the dialog box.
6. Click the table header **Fill**.
   A **Color Spectrum** dialog box appears. Set an appropriate color range by clicking the **Minimum color** and **Maximum color** buttons. When finished, click **OK** to close the dialog box.
7. Click **OK** to close the **Enviroment Options** dialog box.
8. Choose **Animation...** from the **File** menu.
   The **Animation** dialog box appears (Fig. 2.42).
9. Click the **open file** button  .
   A **Save File** dialog box appears. Select or specify a file name in the dialog box, then click **Open**.
10. Check **Create New Frames**, set **Result Type** to Concentration (MT3D) and set **Display Time (s)** to 0.1. **Display Time** is the display duration for each frame.
11. In the **Animation** dialog box, click **OK** to start the animation.

PMWIN will create a frame (image) for each time point at which the simulation results (here: concentration) are saved. Each frame is saved using the filenames *fn.xxx*, where *fn* is the **Frame File** specified in step 9 and *xxx* is the serial number of the frame files. Note that if you have complex DXF-basemaps, the process will be slowed down considerably. When all frames are created, PMWIN will repeat the animation indefinitely until the **Esc** key is pressed.

Once a sequence is created, you can playback the animation at a later time by repeating steps 8 to 11 with **Create New Frames** cleared in step 10. You can also use the **Animator** to playback the sequence.

Note that the number and the size of the image files can be very large. Make sure that there is enough free space on your hard disk. To reduce the file size, you can change the size of the PMWIN window before creating the frames. You may turn off the display of the model grid in the **Environment Options** dialog box so that you don't have the grid cluttering the animation.

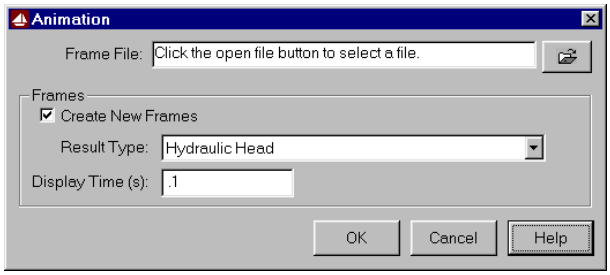


Fig. 2.42 The **Animation** dialog box

3. The Modeling Environment

PMWIN requires the use of **consistent units** throughout the modeling process. For example, if you are using length [L] units of meters and time [T] units of seconds, hydraulic conductivity will be expressed in units of [m/s], pumping rates will be in units of [m^3/s] and dispersivity will be in units of [m].

A toolbar with buttons representing **PMWIN** operations or commands is displayed below the menus. The toolbar is a shortcut for the pull-down menus. To execute one of these shortcuts, move the mouse cursor over the toolbar button and click on it. In the following sections, the use of the respective menus will be described in detail. Some of this information has already been given in Chapter 2, however, this chapter is a complete reference of all menus and dialogs in **PMWIN**, therefore some repetitions may occur.

PMWIN contains the following menus **File**, **Grid**, **Parameters**, **Models**, **Tools**, **Value**, **Options** and **Help**. The **Value** and **Options** menus are available only in the **Grid Editor** and **Data Editor** environment. **PMWIN** uses an intelligent menu system to help you control the modeling process. If you have specified a model data set, the corresponding item of the **Grid**, **Parameters** and **Models** menus will be checked. To deactivate a selected item in the Models menu, just seleted the item again. If you do not know which model data still need to be specified, you may try to run your model by selecting the menu item **Run...** from the corresponding model in the **Models** menu. **PMWIN** will then tell you what parameters or model data are necessary to run your model, if unspecified. An overview of the menus in **PMWIN** is given in table 3.1.

Most of the user-specified data are saved in binary files. A list of the internal data files of **PMWIN** is given in Appendix 4. Prior to running the supported models MODFLOW, MT3D, MT3DMS, MOC3D or the inverse models PEST and UCODE, **PMWIN** will generate the required ASCII input files. The names of the ASCII input files are given in Appendix 3. The formats of the input files of MODFLOW and MT3D, MT3DMS and MOC3D can be found in the user's guide the corresponding software on the companion CD-ROM. The particle tracking model PMPATH retrieves the binary data files of **PMWIN** directly, thus no ASCII input file is required by PMPATH.

Table 3.1 An overview of the menus in **PMWIN**

Menu	Description
File	Create new models; open existing models; convert models to the **PMWIN** format; Save and print plots.
Grid	Generate or modify the size of a model grid; input of the geometry of the aquifer.
Parameters	Input of spatial aquifer parameters, for example transmissivity; Input of temporal parameters, for example simulation length or number of stress periods.
Models	Specify model-specific data using the module provided and call simulation programs. For example, you can add wells, use the recharge or river modules to MODFLOW or define the advection or dispersion parameters in MT3D. The simulation programs are called by selecting **Run...** from the corresponding model.
Tools	Call the modeling tools.
Value	Manipulate model data; read or save model data in separate files.
Options	Modify the appearance of the model grid on the screen; Load site maps.
Help	Call the Help file.

3.1 The Grid Editor

The first steps in the groundwater modeling process are to define the goals of the model, select a computer code (here: MODFLOW), collect the necessary data, develop a conceptual model of the groundwater system and define the spatial discretization of the model domain. Anderson and Woessner (1992) discuss the steps in going from aquifer systems to a numerical model grid. Zheng and Bennett (1995) describe the design of model grids which are intended for use both in flow and transport simulations. These sources provide valuable general information relating to spatial discretization and grid design in numerical groundwater modeling.

In the block-centered finite difference method, an aquifer system is replaced by a discretized domain consisting of an array of nodes and associated finite difference blocks (cells). Fig. 3.1 shows a spatial discretization of an aquifer system with a mesh of cells and nodes at which hydraulic heads are calculated. The nodal grid forms the framework of the numerical model. Hydrostratigraphic units can be represented by one or more model layers. The thicknesses of each model cell and the width of each column and row can be specified. The locations of cells are described in terms of columns, rows, and layers. **PMWIN** uses an index notation [J, I, K] for locating the cells. For example, the cell located in the 2nd column, 6th row, and the first layer is denoted by [2, 6, 1].

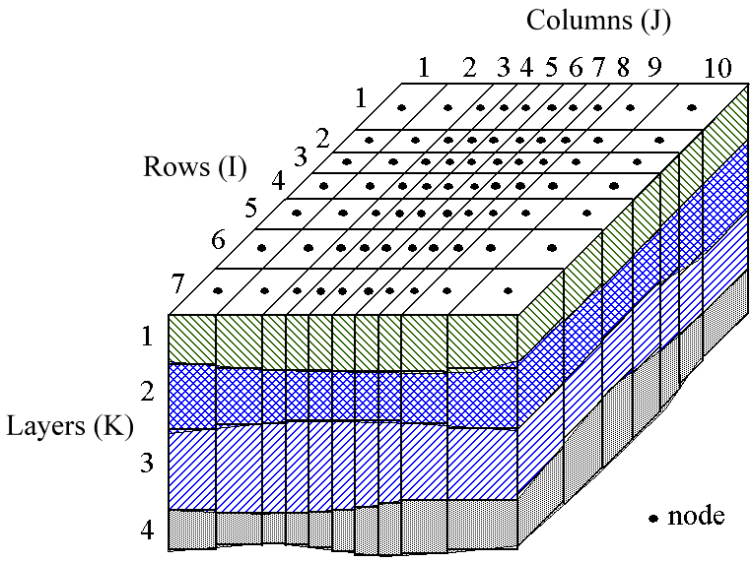


Fig. 3.1 Spatial discretization of an aquifer system and the cell indices

To generate or modify a model grid, choose **Mesh Size...** from the **Grid** menu. If a grid does not exist, a **Model Dimension** dialog box (Fig. 3.2) will allow you to specify the number of layers and the numbers and the widths of columns and rows of the model grid. After specifying these data

and clicking the **OK** button, the **Grid Editor** shows a **worksheet** with a plan view of the model grid (Fig. 3.3). Using the **Environment Options** dialog box (see section 3.9), you can adjust the **coordinate system,** the extent of the worksheet and the positon of the model grid to fit the real-world coordinates of your study site. By default, the origin of the coordinate system is set at the lower-left corner of the worksheet and the extent of the worksheet is set to twice that of the model grid.

The first time you use the **Grid Editor**, you can insert or delete columns or rows (see below). After leaving the **Grid Editor** and saving the grid, you can subsequently refine the existing model grid by calling the **Grid Editor** again. In each case, you can change the size of any column or row. If the grid is refined, all model parameters are retained. For example, if the cell of a pumping well is divided into four cells, all four cells will be treated as wells and the sum of their pumping rates will be kept the same as that of the previous single well. The same is true for hydraulic conductance of the head-dependent boundaries, i.e., river, stream, drain and general-head boundary. If the Stream-Routing Package is used, you must redefine the segment and reach number of the stream.

- **To change the width of a column and/or a row**

1. Click the **assign value** button  .
   The grid cursor appears only if the Assign Value button is pressed down. You do not need to click this button, if its relief is already sunk, ie, if it is already active.
2. Move the grid cursor to the desired cell by using the arrow keys or by clicking the mouse on the desired position. The sizes of the current column and row are shown on the status bar.
3. Press the right mouse button once.
   The **Grid Editor** shows a **Size of Column and Row** dialog box (Fig. 3.4).
4. In the dialog box, type new values, then click **OK**.

- **To insert or delete a column and/or a row**

Inserting or deleting columns/rows is only possible when using the **Grid Editor** for the first time.

1. Click the **assign value** button  .
2. Move the grid cursor to the desired cell by using the arrow keys or by clicking the mouse on the desired position.
3. Hold down the **Ctrl-key** and press the **up** or **right** arrow key to insert a row or a column;. press the **down** or **left** arrow key to delete the current row or column.

- **To refine a column and/or a row**

Refining columns/rows is only possible when the grid has already been saved.

1. Click the **assign value** button .
2. Move the grid cursor to the desired cell by using the arrow keys or by clicking the mouse on the desired position.
3. Hold down the **Ctrl-key** and press the **up** or **right** arrow key to refine a row or a column; press the **down** or **left** arrow key to remove the refinement. The refinements of a column or a row are shown on the status bar.

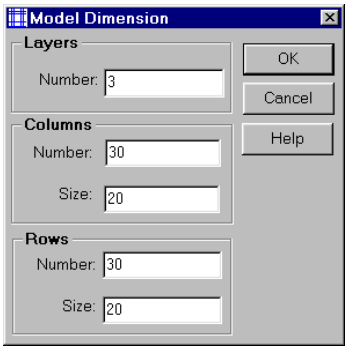


Fig. 3.2 The **Model Dimension** dialog box

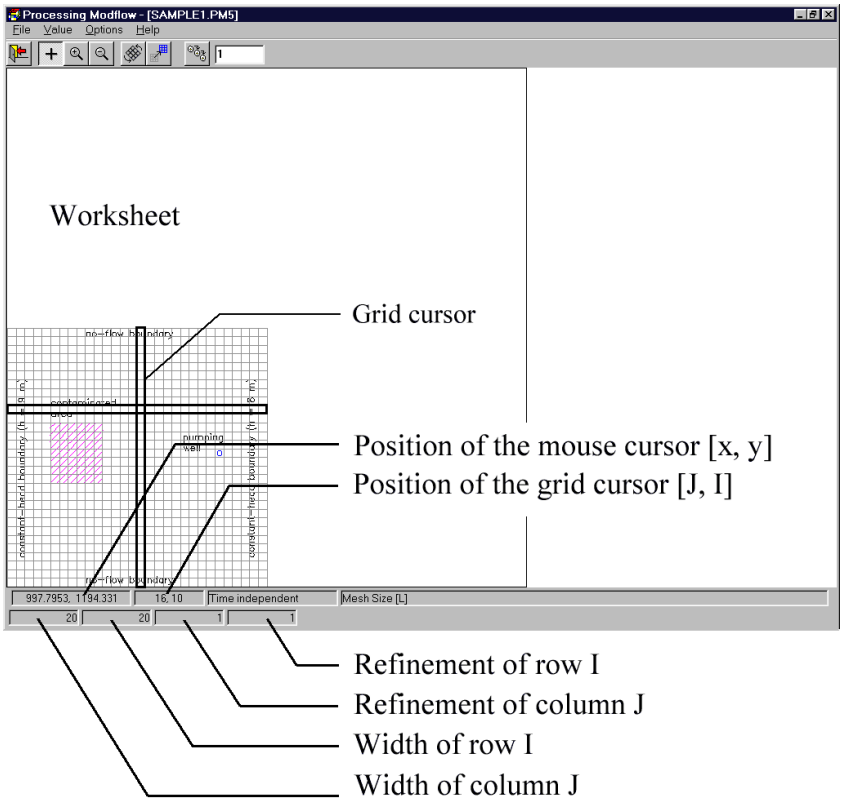


Fig. 3.3 The **Grid Editor**

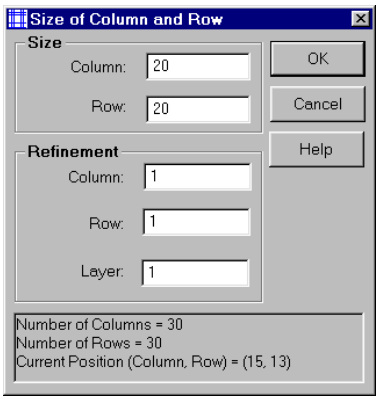


Fig. 3.4 The **Size of Column and Row** dialog box

The following table summarizes the use of the tool bar buttons of the **Grid Editor**.

Table 3.2 Summary of the tool bar buttons for the **Grid Editor**

Button	Action
	**leave editor**; Leave the **Grid Editor**
	**assign value**; Allows you to move the grid cursor and assign values
	**zoom in**; Allows you to drag a zoom-window over a part of the model domain.
	**zoom out**; Displays the entire worksheet.
	**rotate grid**; To rotate the model grid, click the mouse on the worksheet and hold down the left button while you move the mouse.
	**shift grid**; To shift the model grid, click the mouse on the worksheet and hold down the left button while you move the mouse.
	**duplication on/off**; If **duplication** is turned on, the size of the current row or column will be copied to all rows or columns passed by the grid cursor. **Duplication** is on, when the relief of the button is sunk.

3.2 The Data Editor

The **Data Editor** is used to assign parameter values to the model cells. To start the **Data Editor**, select a corresponding item from the **Grid**, **Parameters** or **Models** menu. For example, if you want to assign horizontal hydraulic conductivity to model cells, you will choose **Horizontal Hydraulic Conductivity** from the **Parameters** menu.

The **Data Editor** provides two display modes - **local** and **real-world**, and two input methods - **cell-by-cell** and **zonal**. In the **local display** mode, the display is zoomed to the model grid as shown in Fig. 3.5. In the **real-world display** mode, the entire worksheet is displayed (Fig. 3.6). Similar to the the **Grid Editor**, you can adjust the **coordinate system,** the extent of the **worksheet** and the positon of the model grid to fit the real-world coordinates of your study site by using the **Environment Options** dialog box (see section 3.9). Regardless of the choice of the display modes, the mouse position ([x, y] in the status bar) is always expressed in the real-world coordinates.

When the Data Editor is loaded, it displays the plan view of the first model layer. You can move to another layer by pressing PgDn or PgUp keys or click the **Current Layer** edit field in the tool bar, type the new layer number, and press **Enter**. A summary of the tool bar buttons is given in the table 3.3.

Table 3.3 Summary of the tool bar buttons for the **Data Editor**

Button	Action
	Leave the **Data Editor**.
	**assign value**; Allows you to move the grid cursor and assign values.
	**zoom in**; Allows you to drag a zoom-window over a part of the model domain.
	**zoom out**; Displays the entire worksheet.
	**Cell-by-cell input method**; Switch to the cell-by-cell input method.
	**Zone input method**; Switch to the zone input method.
	**local display mode**; Switch to the local display mode.
	**real-world display mode**; Switch to the real-world display mode.
	**duplication on/off**; If **duplication** is turned on, the cell value(s) of the current cell will be copied to all cells passed by the grid cursor. **Duplication** is on, when the relief of the button is sunk.
	**layer copy on/off**; If you turn **layer copy** on and then move to another layer, the zones and cell values of the current layer will be copied. **Layer copy** is on, when the relief of the button is sunk.

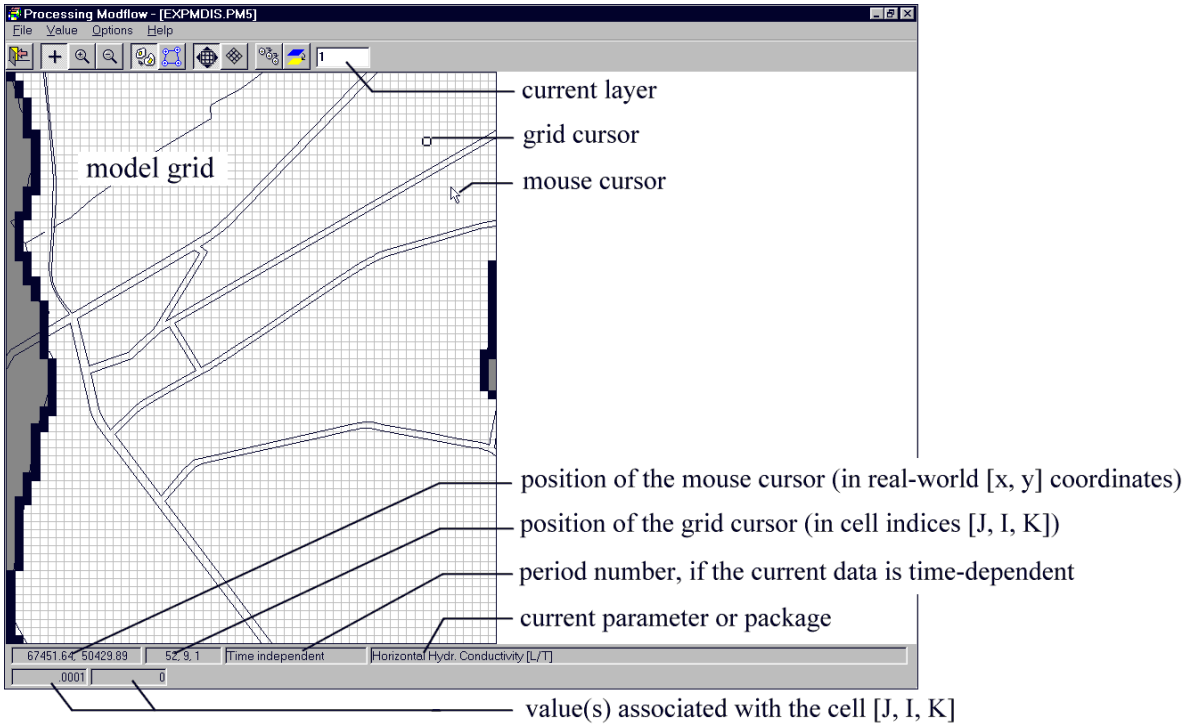


Fig. 3.5 The **Data Editor** (local display mode)

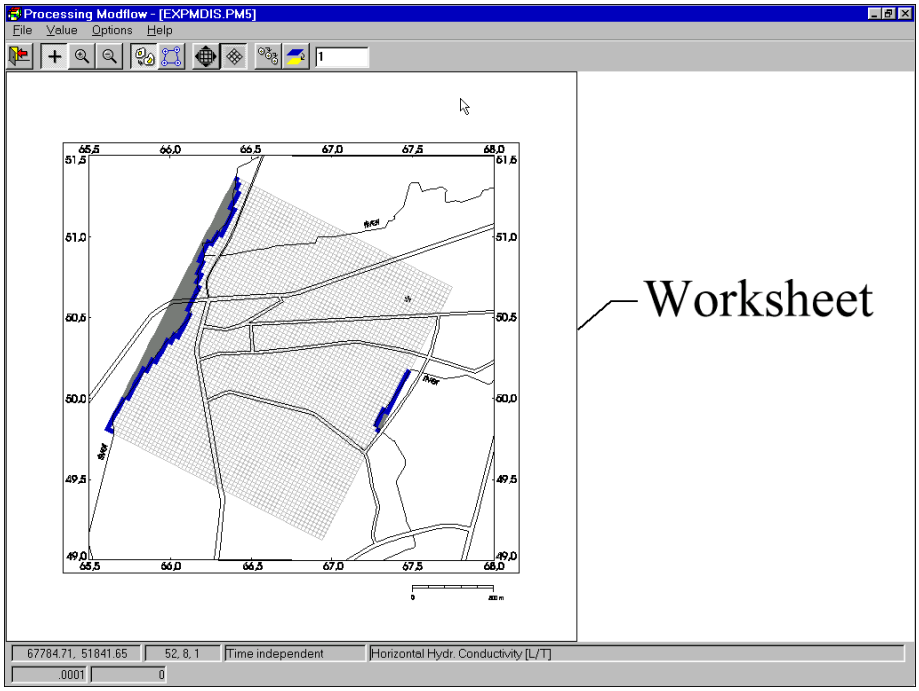


Fig. 3.6 The **Data Editor** (real-world display mode)

3.2.1 The Cell-by-Cell Input Method

To activate this method, click the **cell-by-cell** button or choose **Input Method ▸ Cell-By-Cell** from the **Options** menu.

▸ **To assign new value(s) to a cell**

1. Click the **assign value** button .
   You do not need to click this button, if its relief is already sunk.
2. Move the grid cursor to the desired cell by using the arrow keys or by clicking the mouse on the cell. The value(s) of the current cell will be shown in the status bar.
3. Press the right mouse button once.
   The **Data Editor** shows a dialog box.
4. In the dialog box, type new value(s) then click **OK**.

▸ **To check/modify cell value(s)**

1. Double-click a cell, the **Data Editor** will highlight the cells that have the same value as the clicked cell.
2. Hold down the **Shift** key and press the left mouse button to open a **Cell Infomation** dialog box (Fig. 3.7) for checking (but not editing) the user-specified data of the cell under the grid cursor.
3. Hold down the **Ctrl** key and press the left mouse button to open a **Search and Modify Cell Values** dialog box (Fig. 3.8). This allows you to display all cells that have a value located within the **Search Range** (to be specified). According to the user-specified **Value** and the operation **Options**, you can easily modify the cell values. For example, if **Add** is used, the user-specified value will be added to the cell value. The **Parameter** drop-down box shows the available parameter type(s). You may select the parameter to which the subsequent **Search and Modfiy** operation will be applied.

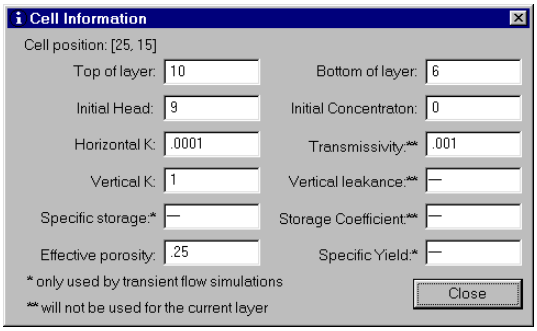


Fig. 3.7 The **Cell Information** dialog box

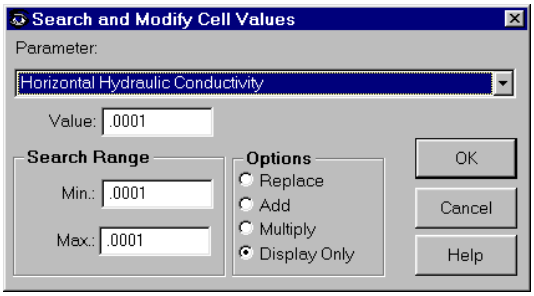


Fig. 3.8 The **Search and Modify Cell Values** dialog box

3.2.2 The Zone Input Method

The Zone Input Method allows you to assign parameter values by zones. To activate this method, choose **Input Method ▸ Zones** from the **Options** menu. Alternatively, you may click on the button . Zones must be designed or drawn first before assigning parameter values to them.

- **To draw a zone**

1. Click the **assign value** button .
   You do not need to click this button, if its relief is already sunk.
2. Click the mouse cursor on a desired position to anchor one end of a line.
3. Move the mouse to another position then press the left mouse button again.
4. Repeat steps 2 and 3 until the zone is closed or press the right mouse button to abort.

- **To delete a zone**

1. Click the **assign value** button .
   You do not need to click this button, if its relief is already sunk.
2. Move the mouse cursor into a zone.
   The boundary of the zone will be highlighted. The value(s) of the current zone will be shown on the status bar.
3. Press the Del-key.

- **To assign new value(s) to a zone**

1. Click the **assign value** button .
   You do not need to click this button, if its relief is already sunk.
2. Move the mouse cursor into a zone.
   The boundary of the zone will be highlighted. The value(s) of the current zone will be shown on the status bar.

3. Press the right mouse button once.
   The **Data Editor** displays a dialog box.
4. In the dialog box, type new value(s) then click  to transfer the new zone value(s) to cells.

> Note that **PMWIN** always uses cell data for computations, and if zone data are not transferred to the grid cells, the original values in the cells are used.

▸ **To modify a zone**

1. You may shift a vertex of a zone by pointing the mouse cursor at the vertex node and pressing down the left mouse button while moving the mouse.
2. If you have several zones, some zones can intersect or even cover other zones. If you move the mouse cursor into a covered zone, the boundary of the zone will not be highlighted. In this case, you can move the mouse cursor into that zone, hold down the Ctrl-key and press the left mouse button once. The **Data Editor** will resort the order of the zones and the "lost" zone will be recovered.

3.2.3 Specification of Data for Transient Simulations

If your model has more than one stress period, a **Temporal Data** dialog box appears after clicking the **leave editor** button  . This dialog box allows you to manage your model data for transient simulations:

1. You can edit model data for a particular stress period by selecting a row of the table and clicking the **Edit Data** button. After having specified the model data of a stress period, the **Data** flag in the corresponding row is checked.
2. You may click on a **Use** flag to check or uncheck it. If the **Use** flag is checked, the data of the corresponding stress period will be used for the flow simulation. If the **Use** flag is not checked, the data of the previous stress period will be used. The **Use** flag of a stress period is automatically deactivated if the corresponding model data are not available.
3. Use Copy Data, if you want to copy model data from one stress period to another.

Fig. 3.9 shows an example in which the data for the periods 1, 3, 4 are specified. The specified data of the first period will be used throughout the first three periods. The data of the fourth period will be used for the rest of the simulation. The data of the third period will not be used because the **Use** flag is cleared.

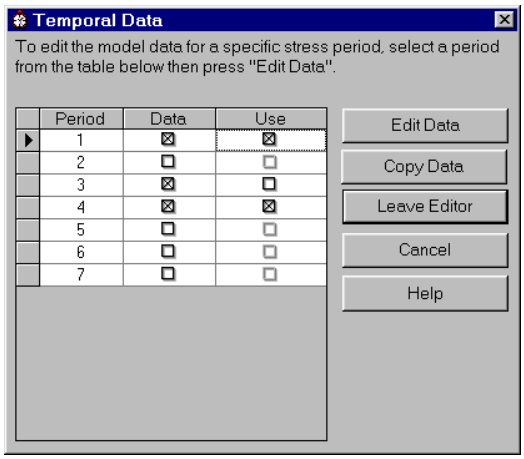


Fig. 3.9 The **Temporal Data** dialog box

3.3 The File Menu

New Model

Select **New Model** to create a new model. A **New Model** dialog box allows you to specify a filename on any available folder or drive for the new model. A **PMWIN** model must always have the file extension **.pm#** (where # is the version number of Processing Modflow). All file names valid under Windows 95/98/NT with up to 120 characters can be used. It is a good idea to save every model in a separate folder, where the model and its output data will be kept. This will also allow you to run several models simultaneously (multitasking).

Open Model...

Use **Open Model...** to load an existing **PMWIN** model. Once a model is opened, **PMWIN** displays the filename of the model on the title bar.

Convert Model...

A **Convert Models** dialog box appears after selecting this menu item. The options in this dialog box are grouped under three tabs - **PMWIN** 4.x, MODFLOW-88/96 and Telescoping Flow Model (Fig. 3.10). Using the first two tabs, you can convert existing **PMWIN** 4.x or MODFLOW models to the format of the present version of **PMWIN**. The use of these two tabs is straightforward. First, click the **open file** button  and select a **PMWIN** *4.x* model or a *MODFLOW Name File* from an **Open** dialog box. Then click the **Convert** button to start the conversion. Refer to Appendix 3 for the definition of *Name Files.*

Telescoping Flow Model (Fig.3.11) allows you to create local-scale submodels from a regional model. To create a submodel, just select an existing **PMWIN** model and specify the subregion. Then click the **Convert** button. The flow simulation of existing **PMWIN** model must be performed. The subregion is given by the starting and ending columns and rows. **PMWIN** automatically transfers the model parameters and the calculated heads from the regional model to the subregional local model. The boundary of the local model will be set to fixed-head boundary (for steady-state simulations) or time-variant specified-head boundary (for transient simulations).

Indenpendent of the selected tab, you can specify refinement factors for both column and row directions. So you can load or create a model with a higher resolution for transport simulations.

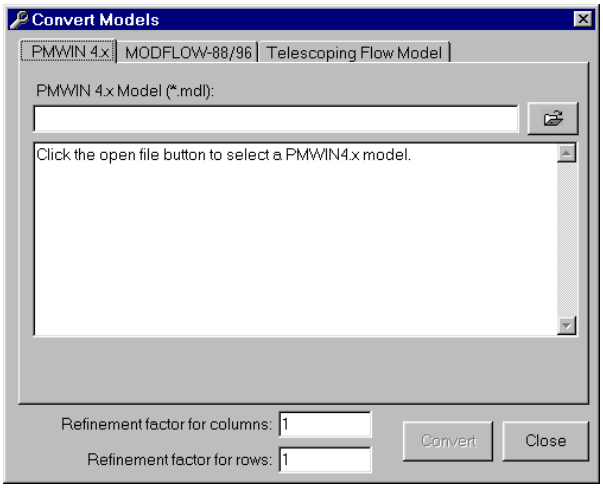


Fig. 3.10 The **Convert Models** dialog box

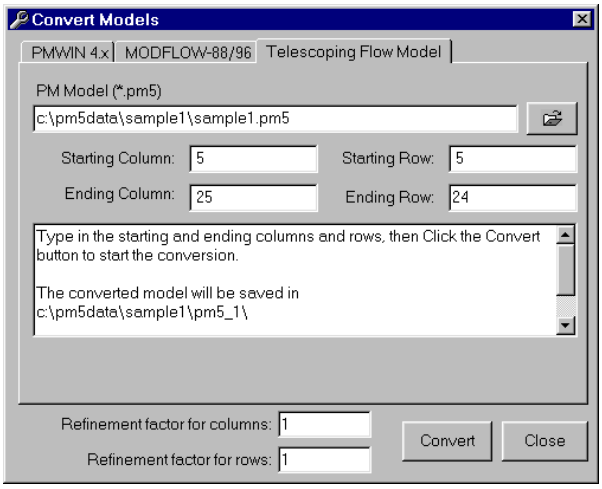


Fig. 3.11 Telescoping a flow model using the **Convert Models** dialog box

Model Information...

The **Model Information** dialog box (Fig. 3.12) provides brief information about your model. You can type a simulation title into the dialog. The maximum length of the simulation title is 132 characters.

Save Plot As...

Use **Save Plot As** to save the contents of the worksheet in graphics files (Fig. 3.13). Three graphics formats are available: Drawing Interchange File (DXF), Hewlett-Packard Graphics Language (HP-GL) and Windows Bitmap (BMP). DXF is a fairly standard format developed by

Autodesk for exchanging data between CAD systems. HP-GL is a two-letter mnemonic graphics language developed by Hewlett-Packard. These graphics formats can be processed by most graphics or word-processing software, and graphics devices.

To save a plot, use the **Format** drop-down box to select a graphic format. Then, enter a filename into the **File** edit field, or click  and select a file from a dialog box. When finished, click OK. Note that for the real-world display mode only the BMP-format can be used.

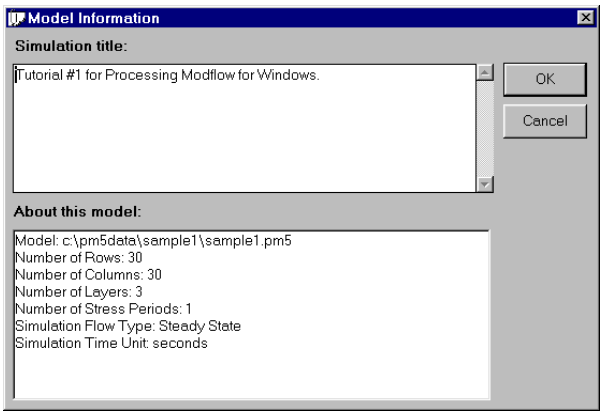


Fig. 3.12 The **Model Information** dialog box

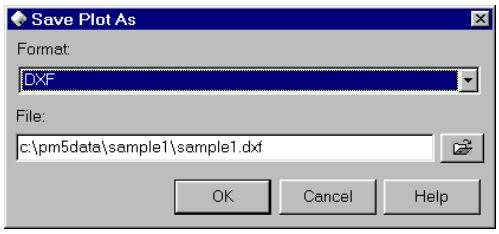


Fig. 3.13 The **Save Plot As** dialog box

Print Plot...

This menu item is only activated in the **Data Editor**. After selecting this item, a **Print Plot** dialog box is displayed with a preview window. The options are described below.

- **Use full page**: The plot is scaled to fit the paper, the original aspect ratio will not be changed.
- **Center on page:** The plot is place on the center of the page.
- **Image Size (millimeters)**: Specify the width and height of the printed image in millimeters.
- **Margins (millimeters):** Specify the left and top margins of the image in millimeters.
- **Printer:** A **Printer** dialog box allows you to select an installed printer and specify the print quality, the paper size, source and orientation and other printing parameters.
- **Print:** Print the contents shown on the preview window.

- **Close:** Close the **Print Plot** dialog box without printing.

Animation...

This menu item is only activated by using the *Presentation* (**Tools▸Presentation**) tool for creating or displaying an animation sequence. Before creating an animation sequence, you should use the **Enivironment Option** and **Maps Option** dialog boxes (refer to the **Options** menu for details) to make sure that the model grid, maps and contours are set properly.

▸ **To create an animation sequence**

1. Select **Animation...** from the **File** menu.
   An **Animation** dialog box appears.
2. In the **Animation** dialog box, click the **open file** button  .
   A **Save File** dialog box appears. Select an existing frame file or specify a new base file name for the frame files in the dialog box, then click **Open**. Like a movie, an animation sequence is based on lots of frames. Each frame is saved by using the filenames *fn.xxx*, where *fn* is the **Frame File** specified above and *xxx* is the serial number of the frame files.

   Note that you cannot save the animation files in the same folder as your model data. So, you need, first, to create a new folder or select another folder for the files.
3. Check or uncheck **Create New Frames**.
   Check **Create New Frames**, if you want to create a new animation sequence. Uncheck it, if you want to playback a saved sequence.
4. Select an appropriate **Result Type** and **Display Time (s)**.
   Five result types are avaliable, including *Hydraulic Head*, *Drawdown*, and *Concentration* calculated by MT3D, MOC3D and MT3DMS. **Display Time** is the display duration for each frame.
5. Select a species from **Species Number**, if the result type is Concentration (MT3DMS).
6. In the **Animation** dialog box, click **OK** to start the animation.
   PMWIN will create a frame (image) for each time point at which the simulation results have been saved. When all frames are created, **PMWIN** will repeat the animation indefinitely until the **Esc** key is pressed.

3.4 The Grid Menu

Mesh Size

Allows you to generate or modify a model grid. See Section 3.1 for how to use the **Grid Editor**.

Layer Type

Select Layer Type to open the **Layer Options** dialog box (Fig. 3.14). The elements of this dialog box are described below.

▸ **Type**

The numerical formulations, which are used by the Block-Centered-Flow (BCF) package to describe groundwater flow, depend on the type of each model layer. The layer types are:

Type 0 The layer is strictly confined. For transient simulations, the confined storage coefficient (specific storage × layer thickness) is used to calculate the rate of change in storage. Transmissivity of each cell is constant throughout the simulation.

Type 1 The layer is strictly unconfined. The option is valid for the first layer only. Specific yield is used to calculate the rate of change in storage for this layer type. During a flow simulation, transmissivity of each cell varies with the saturated thickness of the aquifer.

Type 2 A layer of this type is partially convertible between confined and unconfined. Confined storage coefficient (specific storage × layer thickness) is used to calculated the rate of change in storage, if the layer is fully saturated, otherwise specific yield will be used. Transmissivity of each cell is constant throughout the simulation. Vertical leakage from above is limited if the layer desaturates.

Type 3 A layer of this type is fully convertible between confined and unconfined. Confined storage coefficient (specific storage × layer thickness) is used to calculate the rate of change in storage, if the layer is fully saturated, otherwise specific yield will be used. During a flow simulation, transmissivity of each cell varies with the saturated thickness of the aquifer. Vertical leakage from above is limited if the layer desaturates.

▸ **Anisotropy factor**

The anisotropy factor is the ratio of transmissivity or hydraulic conductivity (whichever is being used) along the I-direction to transmissivity or hydraulic conductivity along the J-direction. The principal axes of the conductivity tensor must be parallel to the I and J-axes of your model grid,

if the anisotropy factor is not equal to 1. Note that anisotropy as used here does not refer to the ratio of horizontal to vertical hydraulic conductivity (see Leakance below)!

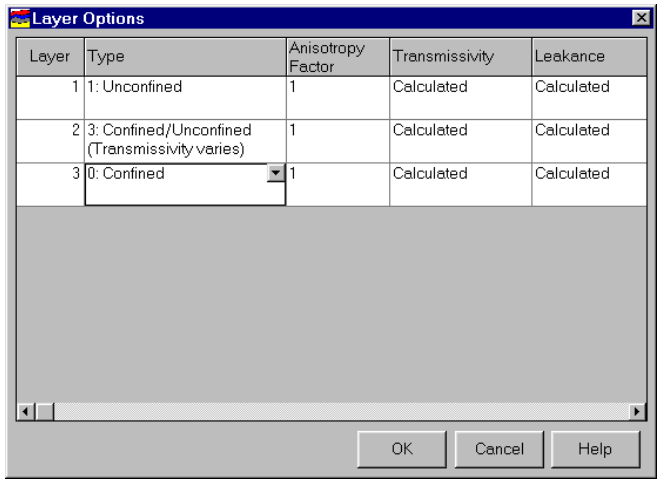


Fig. 3.14 The **Layer Options** dialog box

▸ **Transmissivity**

MODFLOW requires transmissivity (=horizontal hydraulic conductivity [LT^{-1}] × layer thickness [L]) for layers of type 0 or 2. If the Transmissivity flag is set to **Calculated**, **PMWIN** calculates transmissivity by using user-specified horizontal hydraulic conductivity and the elevations of the top and bottom of each layer. Set the Transmissivity flag to **User Specified**, if you want to specify transmissivity manually.

▸ **Leakance**

For flow simulations involving more than one model layer, MODFLOW requires the input of the vertical conductance term, known as vertical leakance (VCONT), between two model layers. Set the Leakance flag of a layer to **User Specified**, if you want to specify the vertical leakance between the layer and the underlaying layer directly. In the **Data Editor**, the vertical leakance between the layers i and i+1 is given as the data of the layer i. A VCONT array is not required for the bottom layer because MODFLOW assumes that the botton layer is underlain by impermeable material. Setting the Leakance flag of a layer to **Calculated** causes **PMWIN** to calculate VCONT by using the following rule.

As illustrated in Fig. 3.15a, when each model layer represents a different hydrostratigraphic unit or when two or more model layers represent a single hydrostratigraphic unit, **PMWIN** uses eq. 3.1 to calculate the vertical leakance VCONT.

$$VCONT = \frac{2}{\frac{\Delta v_k}{(K_z)_{j,i,k}} + \frac{\Delta v_{k+1}}{(K_z)_{j,i,k+1}}} \tag{3.1}$$

where $(K_z)_{j,i,k}$ and $(K_z)_{j,i,k+1}$ are the vertical hydraulic conductivities of layers k and k+1, respectively. While the ratio of horizontal to vertical hydraulic conductivity ranging from 1:1 to 1000:1 is common in model application (Anderson and Woessner, 1992). A summary of hydraulic conductivity values of different materials can be found in Spitz and Moreno (1996).

It is common in applications of MODFLOW to represent the resistance to flow in a low hydraulic conductivity unit (see Fig. 3.15b, semiconfining unit) by lumping the vertical hydraulic conductivity and thickness of the confining unit into a vertical leakance term between the adjacent layers. These kinds of models are often called *quasi three-dimensional models*, because semiconfining units are not explicitly included and simulated. In this case you must manually calculate the VCONT values using eq. 3.2 and enter them into the **Data Editor**.

$$VCONT = \frac{2}{\frac{\Delta z_u}{(K_z)_u} + \frac{2\Delta z_c}{(K_z)_c} + \frac{\Delta z_L}{(K_z)_L}} \tag{3.2}$$

where $(K_z)_u$, $(K_z)_c$ and $(K_z)_L$ are the vertical hydraulic conductivities of the upper layer, semiconfining unit and lower layer, respectively.

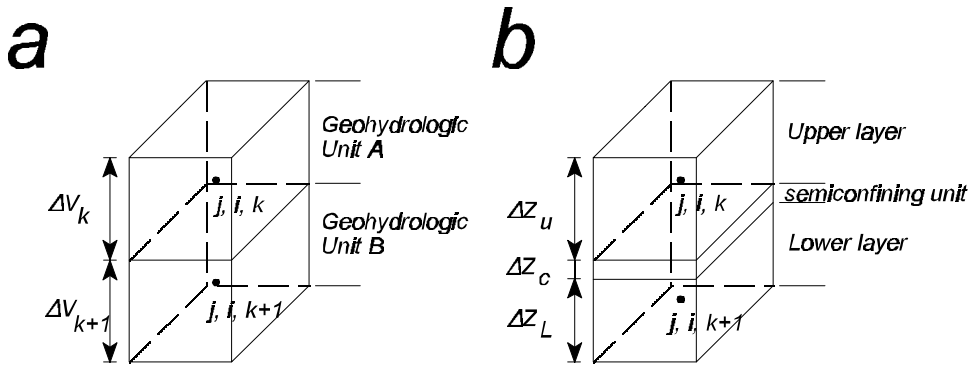


Fig. 3.15 Grid configurations used for the calculation of VCONT

▸ **Storage Coefficient**

For transient flow simulations, MODFLOW requires dimensionless storage terms to be specified for each model layer. For a confined layer, these storage terms are given by the confined storage coefficient (=specific storage [L^{-1}] × layer thickness [L]). If the Storage Coefficient flag is set to **Calculated**, **PMWIN** uses user-specified specific storage coefficients and the elevations of the

top and bottom of each layer to calculate the confined storage coefficient. Set the Storage Coefficient flag to **User Specified**, if you want to specify the confined storage coefficient manually. For an unconfined layer, the storage values are equal to specific yield [-]. The setting of the Storage Coefficient flag has no influence on the specific yield.

▸ Interbed Storage

PMWIN supports the Interbed-Storage package for calculating storage changes from both elastic and inelastic compaction of each model layer. Check the flag of a layer, if you want to use the Interbed-Storage package. see **Models** Menu for details about this package.

▸ Density

Check the flag of a layer, if you want to use the Density package to simulate the effect of density differences on the groundwater flow system. Density-effect can only be applied to layers of type 0 or 2. See **Models** Menu for more information about the **Density** package.

Boundary Condition

▸ IBOUND (Modflow)

An IBOUND array is required by the flow model MODFLOW. The IBOUND array contains a code for each model cell. A positive value in the IBOUND array defines an active cell (the hydraulic head is computed), a negative value defines a fixed-head cell (the hydraulic head is kept fixed at a given value) and the value 0 defines an inactive cell (no flow takes place within the cell). It is suggested to use 1 for active cells, 0 for inactive cells and -1 for fixed-head cells. For fixed-head cells, the initial hydraulic head remains the same throughout the simulation. The initial hydraulic head is specified by choosing Starting **Values ▸ Hydraulic Heads** from the **Parameters** menu. A fixed-head boundary exists whenever an aquifer is in direct hydraulic contact with a river, a lake or a reservoir in which the water level is known. It is important to know that a fixed head boundary provides inexhaustible supply of water. A groundwater system may get as much water as necessary from such a boundary without causing any change in boundary head. In some situations, this may be unrealistic. Therefore care must be taken when using fixed-head boundaries. Consider to use the General-Head Boundary or the Time-Variant Specified-Head packages, if the hydraulic head at the fixed-head boundary varies with time.

If you intend to use the transport model MOC3D, you should be aware that MOC3D allows you to specify *zones* along the fixed head boundaries, which are associated with different source concentrations. *Zones* are defined within the IBOUND array by specifying unique negative values. For example, if you have three zones, you will use -1, -2 and -3 for the fixed-head cells. Note that

the associated concentrations can be specified by selecting **MOC3D ▸ Sink/Source Concentration ▸ Fixed-Head Cells...** from the **Models** menu.

▸ ICBUND (MT3D)

An ICBUND array is required by the transport models MT3D and MT3DMS. ICBUND contains a code for each model cell. A positive value in the ICBUND array defines an active concentration cell (the concentration varies with time and is calculated), a negative value defines a constant-concentration cell (the concentration is constant) and the value 0 defines an inactive concentration cell (no transport simulation takes place at such cells). It is suggested to use the value 1 for an active concentration cell, -1 for a constant-concentration cell, and 0 for an inactive concentration cell. Note that the ICBUND array applies to **all species** if MT3DMS is used.

MT3D and MT3DMS automatically convert no-flow or dry cells to inactive concentration cells. Active variable-head cells can be treated as inactive concentration cells to minimize the area needed for transport simulation, as long as the solute transport is insignificant near those cells. For constant-concentration cells, the initial concentration remains the same at the cell throughout the simulation. A fixed-head cell may or may not be a constant-concentration cell. The initial concentration is specified by choosing **MT3D ▸ Initial Concentration** or **MT3DMS ▸ Initial Concentration...** from the **Models** menu. Note that for multi-species simulation in MT3DMS, the boundary condition type defined by **ICBUND is shared by all species**.

Top of Layers (TOP)

The top elevation of a layer is required when

1. layer type 2 or 3 is used,
2. one of the transport models PMPATH, MT3D, MT3DMS or MOC3D is used,
3. vertical leakance to the underlaying layer is calculated by **PMWIN**, or
4. transmissivity or confined storage coefficient is calculated by **PMWIN** (see Layer Type).

Bottom of Layers (BOT)

The bottom elevation of a layer is required when

1. layer type 1 or 3 is used,
2. one of the transport models PMPATH, MT3D , MT3DMS or MOC3D is used,
3. vertical leakance to the underlaying layer is calculated by **PMWIN**, or
4. transmissivity or confined storage coefficient is calculated by **PMWIN** (see Layer Type).

3.5 The Parameters Menu

Time

Use the **Time Parameters** dialog box (Fig. 3.16) to specify temporal parameters, including the time unit, the length of stress periods and the numbers of stress periods, time steps and transport steps. The table and the elements of this dialog box are described below.

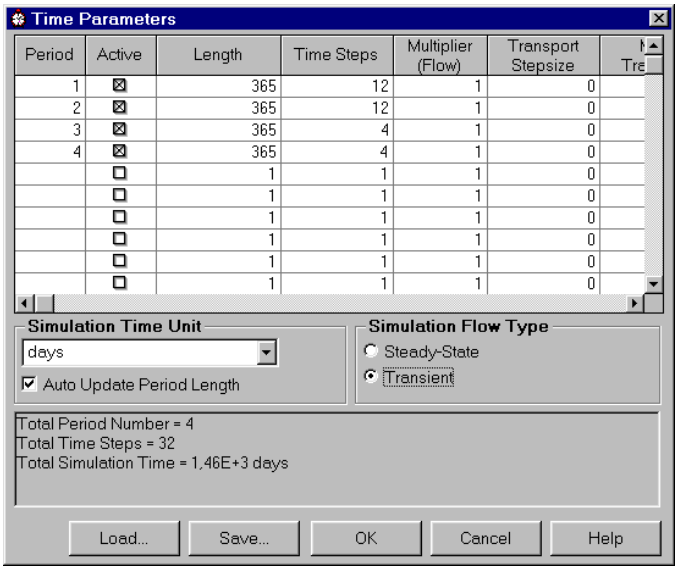


Fig. 3.16 The **Time Parameters** dialog box

- **Period, Active, Length, Time Step**: In MODFLOW, the simulation time is divided into stress periods, which are, in turn, divided into time steps. Check the **Active** flag to activate a stress period. For each stress period, you have the option of changing parameters associated with head-dependent boundary conditions in the River, Stream, Drain, Evapotranspiration, General-Head Boundary and Time-Variant Specified-Head Boundary packages, as well as the recharge rates in the Recharge package and pumping rates in the Well package. For transport simulations, you can change source concentration associated with the fluid sources and sinks. The **length** of stress periods and time steps is not relevant to steady state flow simulations. However, if you want to perform transport simulations at a later time, you must specify the actual period length.
- **Multiplier (FLOW):** MODFLOW allows the time step to increase as the simulation progresses. It uses the following formulae to increase the lengths of time steps as a geometric progression.

$$Delt(1) = \frac{PERLEN \cdot (1 - TSMULT)}{1 - TSMULT^{NSTP}} \tag{3.3}$$

$$Delt(m+1) = TSMULT \cdot Delt(m) \tag{3.4}$$

where PERLEN is the length of a stress period, TSMULT is the time step multiplier, NSTP is the number of time steps and Delt(m) is the length of time step m in a stress period.

- **Transport Step size:** In the transport models MT3D, MT3DMS and MOC3D, each time step is further divided into smaller time increments, called transport steps. Because the explicit numerical solution of the solute-transport equation has certain stability criteria associated with it, the length of a time step used for a flow solution may be too large for a transport solution. Each time step must, therefore, be divided into smaller transport steps.

  For explicit solutions in MOC3D, MT3D or MT3DMS (i.e. when the Generalized Conjugate Gradient solver is not used), the **transport step sizes** in the table are used for the simulation. Considering stability criteria, the transport models always calculate a maximum allowed transport step size Δt_{max}. Setting the transport step size in the table to zero to a value greater than Δt_{max} will cause Δt_{max} to be used for the simulation. For details about the stability criteria associted with the explicit transport-solution, refer to Zheng (1990) or Konikow et al. (1996).

  For implicit solutions in MT3DMS (i.e. when the Generalized Conjugate Gradient solver is used), the **transport step sizes** in the table are the initial transport step size in each flow time step. The subsequent transport stepsize may increase or remain constant depending on the user-specified transport stepsize multiplier (see below). If the transport step size is specified as zero, the model-calculated value, based on the user-specified Courant number in the **Advection Package (MT3DMS)** dialog box, is used.
- **Max. No. of Transport Steps** is used by MT3D and MT3DMS. If the number of transport steps within a flow time step exceeds the maximum number, the simulation is terminated.
- **Multiplier (Transport)** is the multiplier for successive transport steps within a flow time step. This value is only used by MT3DMS for the case that the Generalized Conjugate Gradient solver and the upstream finite-difference method are selected.
- **Simulation Time Unit:** Each time you select a time unit from the **Simulation Time Unit** group, **PMWIN** will update the period length in the table, if **Auto Update Period Length** is checked.
- **Simulation Flow Type: PMWIN** allows you to perform steady state or transient flow simulations by selecting an option from the **Simulation Flow Type** group. You can run a

steady state simulation over several stress periods. In this case, a steady state solution is calculated for each stress period.

- **Save** and **Load**: Using these buttons, you can save or load the contents of the table in or from a time parameter file. The format of the time parameter file is given in Appendix 2.

Initial Hydraulic Heads

MODFLOW requires initial hydraulic heads at the beginning of a flow simulation. Initial hydraulic heads at fixed-head cells will be kept constant during the flow simulation.

For transient flow simulations, the initial heads must be the actual values. For steady-state flow simulations, the initial heads are starting guessed values for the iterative equation solvers. The heads at the fixed-head cells must be the actual values while all other initial heads can be set arbitrarily. For an unconfined layer (layer type 1 or 3), the initial hydraulic head of a fixed-head cell must be higher than the elevation of the cell bottom, because MODFLOW does not convert a dry fixed-head cell to an inactive cell. If any constant-head cell becomes dry, MODFLOW will stop the flow simulation and write a message "CONSTANT-HEAD CELL WENT DRY - SIMULATION ABORTED" into the run record file OUTPUT.DAT.

Both MT3D and MOC3D require initial concentration at the beginning of a transport simulation. Initial concentration at constant-concentration cells will be kept constant during the simulation. Constant-concentration cells can be used to simulate contaminated areas with a fixed concentration. Note that the constant-concentration boundary condition is not implemented in MOC3D.

Boreholes and Observations...

The options of the **Boreholes and Observations** dialog box are grouped under two tabs - **Boreholes** and **Observations**.

- **Boreholes**: The **real-world** coordinates (eastings (x), northings (y)) and the layer number of each borehole are given in the table. A borehole is active if the **Active** flag is checked. While you are editing your model data using the **Data Editor**, active boreholes and the corresponding borehole name can be displayed. After a simulation, **PMWIN** will interpolate the simulation results to the active boreholes. So, you may use the **Graph Viewer** (**Tools▸Graph**) to display the temporal development of a certain result type, for example head-time curves or breakthrough curves. You can also use the **Graph Viewer** to display a scatter diagram for comparing the observed and calculated values.

- **Observations**: The name of the borehole, at which the observations are made, is given in **Borehole name.** The observation time, to which the measurement pertains, is measured from the beginning of the model simulation. You must specify the observation times in ascending order. If you use inverse models PEST or UCODE for calibrating a steady-state flow model with one stress period (you may run a steady-state flow simulation over several stress periods), the length of the period is given as the observation time.

  The **Weight** of an observation gives a relative confidence level of the observed value. The higher the value, the *better* is the measurement. The weight can be set at zero if you wish (meaning that the observation takes no part in the calculation of the objective function during an automatic calibration process), but it must not be negative. Refer to the documentations of UCODE and PEST for the function of weights in the parameter estimation process. Note that drawdown at a certain observation time is defined by $h_0 - h$, where h_0 is the initial hydraulic head and h is the head at the observation time.
- **Save, Load and Clear**: Click the **Clear** button to clear the observation or borehole table. Using the buttons **Save** and **Load**, you can save or load the contents of tables in or from a Borehole file or Observation file. The format of these files is given in Appendix 2.

Note that you can insert or delete a row in a table by pressing the **Ctrl+Ins** or **Ctrl+Del** key. In **PMWIN**, the maximum number of Boreholes is 1000. The maximum number of Observations is 10000.

Horizontal Hydraulic Conductivity and Transmissivity

Horizontal hydraulic conductivity is the hydraulic conductivity along model rows. It is multiplied by an anisotropy factor specified in the **Layer Options** dialog box to obtain the hydraulic conductivity along model columns. Horizontal hydraulic conductivity is required for layers of type 1 or 3. Transmissivity is required for layers of type 0 and 2. Typical values and ranges of horizontal hydraulic conductivity for different types of soils are given in many groundwater textbooks, for example Freeze and Cherry (1979), Spitz and Moreno (1996) and Fetter (1994).

PMWIN uses the horizontal hydraulic conductivity and layer thickness to calculate transmissivity, if the corresponding Transmissivity flag in the **Layer Options** dialog box is **Calculated**. You can also specify transmissivity directly by choosing **Transmissivity** from the **Parameters** menu. The specified transmissivity values of a model layer will be used for simulation, if the Transmissivity flag is **User-specified**. See section 3.4 for more information about the **Layer Options** dialog box.

Vertical Hydraulic Conductivity and Vertical Leakance

As discussed in **Layer Type** above, there are two options to input the required vertical leakance (VCONT) between two model layers.

You can specify the vertical leakance directly by choosing **Vertical Leakance** from the **Parameters** menu. The specified **Vertical Leakance** values of a layer will be used for simulation if the Leakance flag in the **Layer Options** dialog box is **User-specified.** In the **Data Editor**, the vertical leakance between the layers i and i+1 is given as the data of the layer i. The vertical leakance is not required for the layer at the very bottom of the model because MODFLOW assumes that the bottom of the model is underlain by impermeable material.

Note that setting the Leakance flag (in the **Layer Options** dialog box) of a layer to **Calculated** causes **PMWIN** to calculate the vertical leakance by using eq. 3.1.

Effective Porosity

If the total unit volume V of a soil matrix is divided into the volume of the solid portion V_s and the volume of viods V_v, the *porosity* n is defined as $n=V_v/V$. Effective porosity (with the respect to flow through the medium) is normally smaller than porosity, because part of the fluid in the pore space is immobile or partially immobile. This may occur when the flow takes place in a fine- textured medium where adhesion (i.e., the attraction to the solid surface of the porous matrix by the fluid molecules adjacent to it) is important. On a more macroscopic scale the effective porosity also has to accommodate the fact that unresolved conductivity variations lead to a reduction of effective porosity.

Effective porosity is used by transport models, for example PMPATH, MOC3D or MT3D, to calculate the average velocity of the flow through the porous medium. If a dual-porosity system is simulated by MT3DMS, effective porosity should be specified as the portion of total porosity filled with mobile water and the “immobile” porosity is defined through **MT3DMS ▸ Chemical Reaction** of the **Models** menu. A summary of representive porosity values for different soil types can be found in Zheng and Bennett (1995) or Domenico and Schwartz (1990).

Specific Storage, Storage Coefficient and Specific Yield

For transient flow simulations, MODFLOW requires dimensionless storage terms specified for each layer of the model. For a steady state simulation, these menu items are not used and are therefore dimmed.

In a confined layer, the storage term is given by *storativity* **or** *confined storage coefficient* (=specific storage [L^{-1}] × layer thickness [L]). The storativity is a function of the compressibility of the water and the elastic property of the soil matrix. The specific storage or specific storativity is defined as the volume of water that a unit column of aquifer releases from storage under a unit decline in hydraulic head. The specific storage ranges in value from 3.3×10^{-6} [m^{-1}] of rock to 2.0×10^{-2} [m^{-1}] of plastic clay (Domenico, 1972).

The confined storage coefficient is required by layers of type 0, 2 and 3. **PMWIN** uses specific storage and the layer thickness to calculate the confined storage coefficient, if the corresponding Storage Coefficient flag in the **Layer Options** dialog is **Calculated**. By setting the Storage Coefficient flag to **User Specified** and choosing Storage Coefficient from the Parameters menu, you can specify the confined storage coefficient directly.

In a phreatic (an unconfined) layer, the storage term is given by *specific yield* or *drainable porosity*. Specific yield is defined as the volume of water that an unconfined aquifer releases from storage per unit surface area of aquifer per unit decline in the water table. Specific yield is a function of *porosity* (and is not necessarily equal to *porosity*), becuase a certain amount of water is held in the soild matrix and cannot be removed by gravity drainage. Specific yield is required for layers of type 1, 2 and 3. Refer to Spitz and Moreno (1996) for a summary of values of specific yield.

Refer to Bear (1972 , 1979) or Freeze and Cherry (1979) for more information about the storage terms and their definitions.

3.6 The Models Menu

3.6.1 MODFLOW

MODFLOW ▸ Density

Using the Density package (Schaars and van Gerven, 1997), the water density of a "density-layer" may differ from cell for cell. During a flow simulation the density-dependent flows will be adapted into the system of flow equations by correcting the hydraulic heads to equivalent fresh water heads (or reference density heads). It is assumed that the density distribution and the internodal transmissivities remain constant during a flow simulation. Therefore, density layers may only be used in combination with layers of the types 0 or 2 (confined). A density-layer is marked by using the **Layer Options** dialog box. Note that the Density package is not a real density flow model. It is only an approximation which is valid as long as flow processes do not change the salinity distribution considerably.

The density package requires the input of a reference density (which is normally set to the density of freshwater) and the density distribution within the density-layers. These values are specified by using the **Data Editor**:

- Reference density (REFRHO) [ML^{-3}] and
- Cell-Density [ML^{-3}].

Note that the Density package is supported only if you select the MODFLOW version "MODFLOW + Density package from KIWA" in the **Run Modflow** dialog box. See **MODFLOW ▸ Run...** for more about the versions of MODFLOW.

MODFLOW ▸ Drain

A drain is defined by using the **Data Editor** to assign three values to a model cell:

- Drain hydraulic conductance (C_d) [L^2T^{-1}],
- Elevation of the Drain (d) [L] and
- Parameter Number [-]

The values C_d and d and the parameter number are shown from left to right on the status bar. The parameter number is used to assign C_d as a parameter for an automatic calibration by the inverse

models PEST or UCODE, see **PEST ▸ Parameter List...** or **UCODE ▸ Parameter List...**. These values are constant during a given stress period. For transient flow simulations involving several stress periods, these values can be different from period to period.
When the hydraulic head (h) in a drain-cell is greater than the drain elevation, water flows into the drain and is removed from the groundwater model. Discharge to the drain is zero when the hydraulic head is lower than or equal to the median drain elevation. Recharge from the drain is always zero, regardless of the hydraulic head in the aquifer. Discharge rate to the drain (Q_d) is calculated by

$$Q_d = C_d \cdot (h - d) \tag{3.5}$$

The value C_d of a drain-cell is often given by

$$C_d = K \cdot L \tag{3.6}$$

where L is the length of the drain within a cell. The value K is an equivalent hydraulic conductivity describing all of the head loss between the drain and the aquifer. It depends on the material and characteristics of the drain itself and the immediate environment. The value C_d is usually unknown and must be adjusted during a model calibration.

MODFLOW ▸ Evapotranspiration

The Evapotranspiration package simulates the effects of plant transpiration and direct evaporation in removing water from the saturated groundwater regime. Evapotranspiration is defined by assigning the following data to each vertical column of cells in the **Evapotranspiration Package** dialog box (Fig. 3.17) of the **Data Editor**:

- Maximum ET Rate R_{ETM} [LT^{-1}],
- Elevation of the ET Surface h_s [L],
- ET Extinction Depth d [L],
- Layer Indicator I_{ET} [-], and
- Parameter Number [-]

The specified values are shown from left to right on the status bar. These values are constant during a given stress period. For transient flow simulations involving several stress periods, these values can be different from period to period. Note that although the values are specified for each vertical column of cells, you may move to other layers within the **Data Editor** and examine the grid configuration in each layer. The parameter number is used to assign R_{ETM} as a parameter for

an automatic calibration by the inverse models PEST or UCODE, see **PEST ▸ Parameter List...** or **UCODE ▸ Parameter List...**.

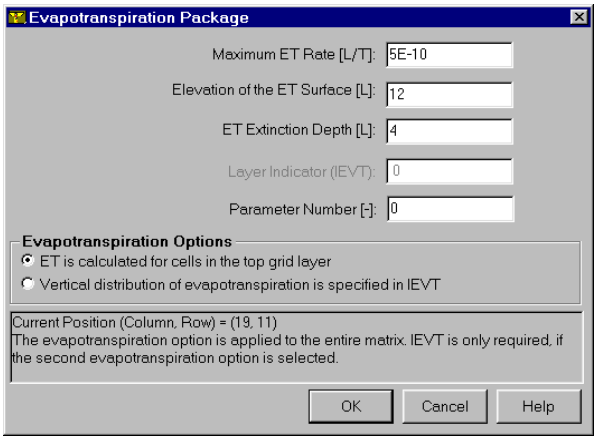


Fig. 3.17 The **Evapotranspiration Package** dialog box

The Evapotranspiration package removes water from the saturated groundwater regime based on the following assumptions:

1. When water table is at or above the elevation of the ET surface h_s, evapotranspiration loss from the water table is at the maximum ET Rate R_{ETM};
2. No evapotranspiration occurs when the depth of the water table below the elevation of the ET surface exceeds the ET extinction depth d; and
3. In between these two extremes evapotranspiration varies linearly with the water table elevation.

These assumptions can be expressed in equation form as:

$$\begin{aligned} R_{ET} &= R_{ETM} && h > h_s \\ R_{ET} &= 0 && h < h_s - d \\ R_{ET} &= R_{ETM} \cdot \left[\frac{h - (h_s - d)}{d} \right] && (h_s - d) \le h \le h_s \end{aligned} \tag{3.7}$$

where R_{ET} [$L^3L^{-2}T^{-1}$] is the evapotranspiration rate per unit surface area of water table. The evapotranspiration flow rate (Q_{ET} [L^3T^{-1}]) drawn from a model cell is

$$Q_{ET} = R_{ET} \cdot DELR \cdot DELC \tag{3.8}$$

where DELR·DELC is the map area of a model cell. Q_{ET} is drawn from only one cell in the vertical column beneath the map area. The Evapotranspiration package provides two options for specifying the cell in each vertical column of cells where evapotranspiration is drawn from:

1. Evapotranspiration is always drawn from the top layer of the model.
2. Vertical distribution of evapotranspiration is specified in the Layer Indicator Array. I_{ET} defines the layer where evapotranspiration is drawn from.

In either case the Q_{ET} has no influence on the simulation if the designated cell is either a no-flow (inactive) cell or a constant head cell. You can select an option in the **Evapotranspiration Package** dialog box. The layer indicator array is needed only when the second option is used.

MODFLOW ▸ General-Head Boundary

The General-Head Boundary package is used to simulate head-dependent flow boundaries (Cauchy boundary conditions). Similar to the Drain package, a General-Head Boundary cell (GHB-cell) is defined by three cell values:

- GHB hydraulic conductance C_b [L^2T^{-1}]
- Hydraulic head at the boundary h_b [L]
- Paramter Number [-]

The parameter number is used to assign C_b as a parameter for an automatic calibration by the inverse models PEST or UCODE, see **PEST ▸ Parameter List...** or **UCODE ▸ Parameter List...**.

Flow through the general-head boundary Q_b [L^3T^{-1}] is calculated by

$$Q_b = C_b (h_b - h) \tag{3.9}$$

where h is the hydraulic head in the aquifer. A GHB-cell is equivalent to a constant head cell, if a very large C_b is used. The values C_b and h_b are constant during a given stress period. For transient flow simulations involving several stress periods, these values can be different from period to period. This allows you to change the head at "constant-head" boundaries as the transient simulation progresses.

MODFLOW ▸ Horizontal-Flow Barrier

The Horizontal-Flow Barrier package simulates thin low-permeability geologic features, such as vertical faults or slurry walls, that impede the horizontal flow of groundwater. These geologic features are approximated as a series of horizontal-flow barriers conceptually situated on the boundaries between pairs of adjacent cells in the finite-difference grid. Refer to Hsieh and Freckleton (1993) for the numerical implementation of the Horizontal-Flow Barrier package.

A horizontal-flow barrier is defined by assigning the following values to a model cell in the **Horizontal-Flow Barrier Package** dialog box (Fig. 3.18):

- Barrier Direction [-]; and
- (Hydraulic Conductivity/Thickness) of the barrier TDW [T^{-1}] for unconfined layers or (Transmissivity/Thickness) of the barrier TDW [LT^{-1}] for confined layers.

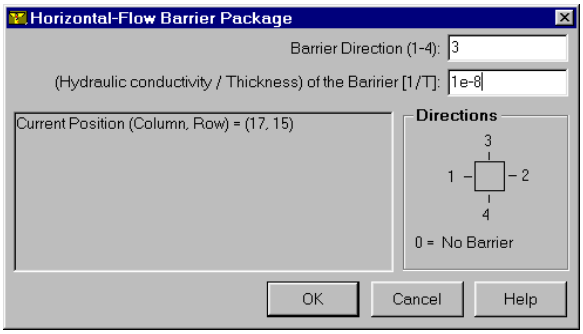


Fig. 3.18 The **Horizontal-Flow Barrier Package** dialog box

The barrier direction indicates the cell face where the barrier is located. To erase an existing barrier, use zero for the barrier direction. The second value TDW gives the hydraulic characteristic of the barrier. If a layer is unconfined (type 1 or 3), TDW is the barrier hydraulic conductivity divided by the thickness of the barrier. If a layer is confined (type 0 or 2), TDW is the barrier transmissivity divided by the thickness of the barrier. The barrier thickness is included implicitly in TDW.

MODFLOW ▸ Interbed Storage

For steady state flow simulations, this menu item is not used and is therefore dimmed.

Groundwater is released from storage under conditions of decreasing hydraulic head. The released water volume is proportional to the compressibility of the soil matrix and water, because a

reduction of the hydraulic head results in an increase in the effective stress on the soil skeleton and a decrease of the water pressure. Increasing effective stress on the soil skeleton results to deformation (compaction) of the soil matrix. The Interbed Storage package (Leake and Prudic, 1991) calculates the water volume released from storage and simulates elastic and inelastic compaction of compressible fine-grained beds in an aquifer due to groundwater extraction. The term "interbed" is used to denote a poorly permeable bed within a relatively permeable aquifer (Fig. 3.19). The interbeds are assumed to consist primarily of highly compressible clay and silt beds from which water flows vertically to adjacent coarse-grained beds.

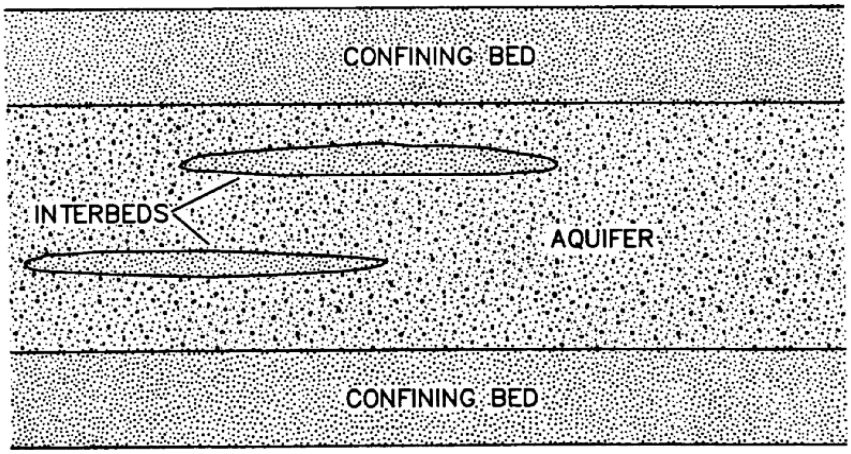


Fig. 3.19 Types of fine-grained beds in or adjacent to aquifers. Beds may be discontinuous interbeds or continuous confining beds. Adopted from (Leake and Prudic, 1991).

To incorporate the calculation of interbed storage of a layer, check the **Interbed Storage** flag in the **Layer Options** dialog box (see section 3.4). The required data are specified by using the **Interbed Storage Package** dialog box of the **Data Editor**.

- **Preconsolidation Head or preconsolidation stress H_c [L]**: Preconsolidation head is the previous minimum head value in the aquifer. For any model cells in which the specified preconsolidation head is greater than the initial hydraulic head, the value of the preconsolidation head will be set to that of the initial hydraulic head;
- **Elastic Storage Factor S_{fe} [-]** for interbeds present in the model layer;
- **Inelastic Storage Factor S_{fv} [-]** for interbeds present in the model layer;
- **Starting Compaction [L]**. Compaction values computed by the Interbed-Storage package are added to the starting compaction so that stored values of compaction and land subsidence may include previous components. The starting compaction does not affect calculations of storage changes or resulting compaction; and

- **Parameter Number [-]**. The parameter number is used to assign S_{fv} as a parameter for an automatic calibration by the inverse models PEST or UCODE, see **PEST ▸ Parameter List...** or **UCODE ▸ Parameter List...**.

For a confined aquifer, elastic compaction or expansion of sediments is proportional or nearly proportional to change in hydraulic head in the aquifer. The following equation is used to calculate the change in the thickness Δb [L] of the interbed (positive for compaction and negative for expansion):

$$\Delta b = -\Delta h \cdot S_{ske} \cdot b_0 = -\Delta h \cdot S_{fe} \tag{3.10}$$

where Δh [L] is change in hydraulic head, positive for increase; S_{ske} [L^{-1}] is the skeletal component of elastic specific storage; b_0 is the thickness of the interbed; and S_{fe} is the user-specified elastic storage factor. When compressible fine-grained sediments are stressed beyond a previous maximum stress (preconsolidation stress), compaction is permanent (inelastic). In analogy to eq. 3.10, the package uses the following equation to calculate the approximate inelastic compaction Δb^* [L]:

$$\Delta b^* = -\Delta h \cdot S_{skv} \cdot b_0 = -\Delta h \cdot S_{fv} \tag{3.11}$$

where S_{skv} [L^{-1}] is the skeletal component of inelastic specific storage and S_{fv} is the user-specified inelastic storage factor.

Elastic compaction or expansion of sediments in an unconfined aquifer can be expressed as

$$\Delta b = -\Delta h \cdot (1 - n + n_w) \cdot S_{ske} \cdot b_0 = -\Delta h \cdot S_{fe} \tag{3.12}$$

where n [-] is porosity and n_w [-] is moisture content above water table as a fraction of total volumn of porous medium. Similarly, inelastic compaction or expansion of sediments can be expressed as

$$\Delta b = -\Delta h \cdot (1 - n + n_w) \cdot S_{skv} \cdot b_0 = -\Delta h \cdot S_{fv} \tag{3.13}$$

For an aquifer with n interbeds with specific-storage values S_{s1}, S_{s2},..., S_{sn} and with thicknesses b_1, b_2, ..., b_n, a single equivalent storage factor S_{sytem} [-] is given by Jorgenson (1980):

$$S_{system} = S_{s1} b_1 + S_{s2} b_2 + \ldots + S_{sn} b_n \tag{3.14}$$

MODFLOW ▸ Recharge

The Recharge package is designed to simulate areally distributed recharge to the groundwater system. Recharge is defined by assigning the following data to each vertical column of cells in the **Recharge Package** dialog box (Fig. 3.20) of the **Data Editor**:

- Recharge Flux I_R [LT^{-1}]
- Layer Indicator I_{RCH} [-]
- Parameter Number [-]

After specifying the values, they are displayed from left to right on the status bar. The parameter number is used to assign the Recharge Flux I_R as a parameter for an automatic calibration by the inverse models PEST or UCODE, see **PEST ▸ Parameter List...** or **UCODE ▸ Parameter List...**. Note that although these values are specified for each vertical column of cells, you may move to other layers within the **Data Editor** and examine the grid configuration in each layer.

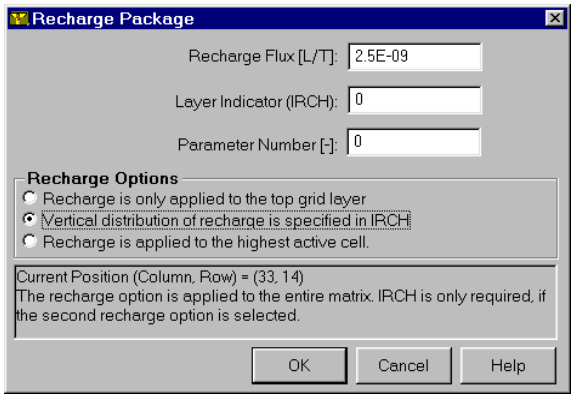


Fig. 3.20 The **Recharge Package** dialog box

MODFLOW uses I_R to calculate the recharge flow rate (Q_R [L^3T^{-1}]) applied to the model cell:

$$Q_R = I_R \cdot DELR \cdot DELC \qquad (3.15)$$

where DELR · DELC is the map area of a model cell. In MODFLOW, the recharge rate Q_R is applied to a single cell within a vertical column of cells. In the simplest situation, the water table is located in the top layer of the model, the top layer is designated as unconfined and an array of Recharge Flux I_R is specified for that layer. Problems may arise, when the water table cuts across layers. To solve this kind of problems, the Recharge package provides three options for specifying the cell in each vertical column of cells that receives the recharge:

1. Recharge is only applied to the top grid layer.
2. Vertical distribution of recharge is specified in the Layer Indicator array I_{RCH}, which defines the layer where recharge is applied.
3. Recharge is applied to the highest active cell in each vertical column. The user does not have to predetermine the layer to which recharge should be applied. The appropriate layer is automatically selected by the Recharge package. If the highest active cell is a constant-head cell recharge will be intercepted and cannot go deeper.

Refer to the description of the Recharge package in McDonald and Harbaugh (1988) for an example of using these options.

MODFLOW ▸ Reservoir

The Reservoir package (Fenske et. al, 1996) is designed for cases where reservoirs are much greater in area than the area represented by individual model cells. More than one reservoir can be simulated using this package. The area subject to inundation by each reservoir is specified by entering the reservoir number for selected cells. For reservoirs that include two or more areas of lower elevation separated by areas of higher elevation, the filling of part of the reservoir may occur before spilling over to an adjacent area. The package can simulate this process by specifying two or more reservoirs in the area of a single reservoir.

Reservoirs are defined by using the **Reservoir Package** dialog box (Fig. 3.21) of the **Data Editor** to assign the following values to the model cells:

- Reservoir Number I_{RES} [-],
- Land-surface elevation of the reservoir B_{RES} [L],
- Vertical hydraulic conductivity of the reservoir bed HC_{RES} [L/T],
- Thickness of the reservoir bed Rb [L], and
- Layer Indicator IRESL [-]
- Parameter Number [-].

The parameter number is used to assign HC_{RES} as a parameter for an automatic calibration by the inverse models PEST or UCODE, see **PEST ▸ Parameter List...** or **UCODE ▸ Parameter List...**.

The elevation of the water table in reservoirs are specified by using the **Stage-Time Table of Reservoirs** dialog box (see below). The land-surface elevation within the specified area of potential inundation for each reservoir is typically defined by the average land-surface elevation

of individual cells within the area. At cells in which reservoir stage exceeds land-surface elevation within the specified reservoir area, the reservoir boundary is activated. Similarly, wherever reservoir stage is less than the land-surface elevation of a cell, the reservoir boundary is not activated. If reservoir stage drops below the lowest land-surface elevation for all cells within the specified reservoir area, water exchange is not simulated between the reservoir and the underlying groundwater system.

In active cells, water exchange between surface water and groundwater is computed in a manner identical to the River package (see below). The Reservoir package is ideally suited for cases where leakage from or to reservoirs may be a significant component of flow in a groundwater system; however, if reservoir stage is unknown, then a more complex conceptualization would be needed in which reservoir stage would be computed as part of the simulation rather than having stage specified as model input. For reservoirs where stage is unknown, a program that computes the stage in lakes based on inflows and outflows has been written by Cheng and Anderson (1993).

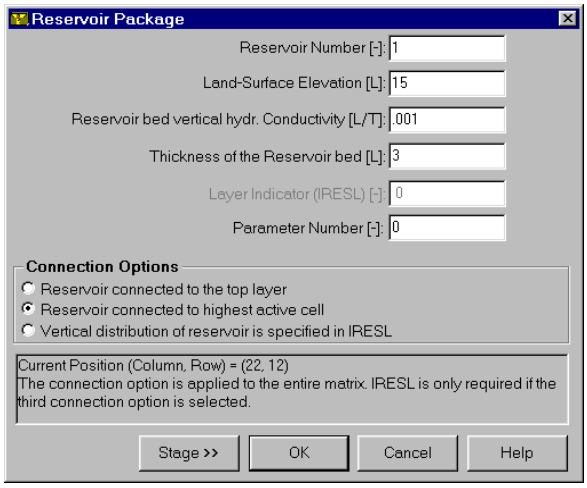


Fig. 3.21 The **Reservoir Package** dialog box

Three options are avaliable for simulating leakage between a reservoir and the underlying groundwater system. The first option simulates leakage only to layer 1; the second option simulates leakage to the uppermost active cell; and the third option simulates leakage to a specified layer for each active reservoir cell. Inherent in the simulation of reserviors is that the reservoir only partially penetrates an active model cell. If the reservoir fully penetrates a cell, the reservoir leakage will be simulated in a lower cell. Thus, water exchange between the groundwater system and the reservoir takes place across the bottom of the reservoir and the top of the model cells.

Leakage between the reservoir and the underlying groundwater system is simulated for each model cell corresponding to the inundated area by multiplying the head difference between the reservoir and the groundwater system by the hydraulic conductance of the reservoir bed. Hydraulic conductance of the reservoir bed is given by eq. 3.16.

$$C_{RES} = HC_{RES} \cdot DELC(I) \cdot DELR(J) \; / \; Rb \qquad (3.16)$$

where DELC(I) is the width of the model row I, DELR(J) is the width of the model column J.

Reservoir bed thickness is substracted from the land-surface elevation of the reservoir to obtain the elevation of the base of the reservoir-bed sediments. The elevation of the base of the reservoir-bed sediments is used in computing leakage. When the head in the groundwater system is above the base of the reservoir-bed sediments, leakage Q_{RES} [L^3T^{-1}] from or to the groundwater system is computed by eq. 3.17.

$$Q_{RES} = C_{RES} \cdot (H_{RES} - h) \qquad (3.17)$$

where H_{RES} is the reservoir stage [L] and h is the groundwater head [L]. When the head in the groundwater system is less than elevation of the base of the reservoir-bed sediments, leakage from the reservoir to the groundwater system is computed by:

$$Q_{RES} = C_{RES} \cdot (H_{RES} - H_{RESBOT}) \qquad (3.18)$$

where H_{RESBOT} is the elevation of the base of the reservoir-bed sediments.

▸ **To specify the stages of reservoirs**

1. Click the **Stage** button from the **Reservoir Package** dialog box (Fig. 3.21).
   A **Stage-Time Table of Reservoirs** dialog box appears (Fig. 3.22).
2. Select a reservoir number (a row) from the first table.
   The reservoir number is corresponding to the number I_{RES} (see above). The description column is a place for you to take notice.
3. Type the observation time and the corresponding stage into the second table.
   The observation time is measured from the start of the model simulation, to which the measured stage pertains.

The Reservoir package requires the input of the starting and ending stages for each stress period. These values are automatically determined by linear interpolation using the values specified in the **Stage-Time Table of Reservoirs** dialog box. If the starting time or the ending time is beyond the latest observation time, the latest observed stage will be used.

Reservoir stage is used to determine whether the reservoir boundary is activated for a model cell at the beginning of each time step. The reservoir stage for each time step is, once again, determined by linear interpolation using the starting and ending stages for the stress period. The interpolated reservoir stage corresponds with the simulation time at the end of a model time step.

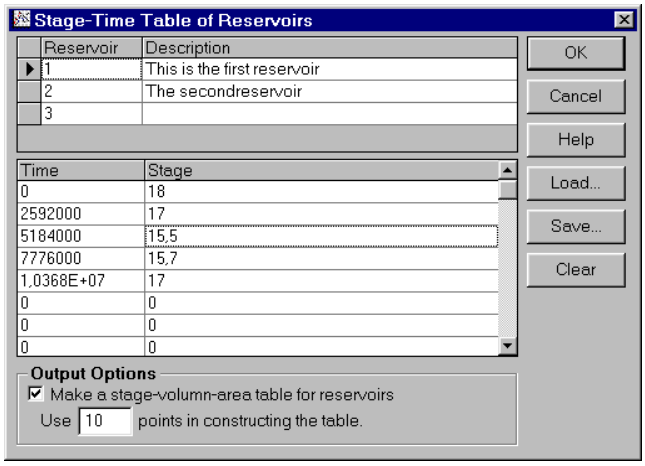


Fig. 3.22 The **Stage-Time Table of Reservoirs** dialog box

MODFLOW ▸ River

The River package is used to simulate the flow between an aquifer and a surface-water feature, such as rivers, lakes or reservoirs. Rivers are defined by using the **River Package** dialog box of the **Data Editor** to assign the following values to the model cells:

- Hydraulic conductance of the riverbed (C_{RIV}) [L^2T^{-1}]
- Head in the river (H_{RIV}) [L],
- Elevation of the bottom of the riverbed (R_{BOT}) [L], and
- Parameter Number [-].

After specifying the values, they are shown from left to right on the status bar. The parameter number is used to assign C_{RIV} as a parameter for an automatic calibration by the inverse models PEST or UCODE, see **PEST ▸ Parameter List...** or **UCODE ▸ Parameter List...**. For transient flow simulations involving several stress periods, these values can be different from period to period. If the hydraulic head (h) in a river-cell is greater than R_{BOT}, the rate of leakage (Q_{RIV}) from the river to the aquifer is calculated by eq. 3.19.

$$Q_{RIV} = C_{RIV} \cdot (H_{RIV} - h) \qquad h > R_{BOT} \tag{3.19}$$

For the case that h is greater than H_{RIV}, Q_{RIV} is negative. It means that water flows from the aquifer into the river and is removed from the groundwater model. When h has fallen below the bottom of the riverbed, the rate of leakage through the riverbed is given by eq. 3.20.

$$Q_{RIV} = C_{RIV} \cdot (H_{RIV} - R_{BOT}) \qquad h \leq R_{BOT} \tag{3.20}$$

The value C_{RIV} of a river-cell is often given by

$$C_{RIV} = \frac{K \cdot L \cdot W}{M} \tag{3.21}$$

where K is the hydraulic conductivity of the riverbed material, L is the length of the river within a cell, W is the width of the river and M is the thickness of the riverbed. If C_{RIV} is unknown, it must be adjusted during a model calibration.

MODFLOW ▸ Streamflow-Routing

The Streamflow-Routing package (Prudic, 1989) is designed to account for the amount of flow in streams and to simulate the interaction between surface streams and groundwater. Streams are divided into segments and reaches. Each reach corresponds to individual cells in the finite-difference grid. A segment consists of a group of reaches connected in downstream order. Streamflow is accounted for by specifying flow for the first reach in each segment, and then computing streamflow to adjacent downstream reaches in each segment as inflow in the upstream reach plus or minus leakage from or to the aquifer in the upstream reach. The accounting scheme used in this package assumes that streamflow entering the modelled reach is instantly available to downstream reaches. This assumption is generally reasonable because of the relatively slow rates of groundwater flow.

Streamflow into a segment that is formed from tributary streams is computed by adding the outflows from the last reach in each of the specified tributary segments. If a segment is a diversion, then the specified flow into the first reach of the segment is subtracted from flow in the main stream. However, if the specified flow of the diversion is greater than the flow out of the segment from which flow is to be diverted, then no flow is diverted from that segment.

In the **Data Editor**, you can press the right mouse button and specify the following required cell values in the **Streamflow-Routine Package** dialog box (Fig. 3.23). The specified cell values will be shown from left to right on the status bar.

- **Segment** is a number assigned to a group of reaches. Segments must be numbered in downstream order. The maximum number allowed in PMWIN is 25.

- **Reach** is a sequential number in a segment that begins with one for the farthest upstream reach and continues in downstream order to the last reach in the segment. In PMWIN, you can only assign one reach to a model cell, although the Streamflow-Routing package allows the user to assign more than one reach in different segments to the same model cell. Refer to the documentation of the **Streamflow-Routing** package (Prudic, 1989) for more information about the numbering scheme.
- **Streamflow** [L^3T^{-1}] is the streamflow entering a segment. This value is specified only for the first reach in each segment. The value is either a zero or a blank when the reach number (Reach) is not 1. When inflow into a segment is the sum of outflow from a specified number of tributary segments, the segment inflow values are specified as -1.
- **Stream Stage** [L] is the head in the stream.
- **Streambed hydraulic conductance** C_{STR}, **Elevation of the Streambed Top** and **Elevation of the Streambe Botton** are used to calculate leakage to or from the aquifer through the streambed. C_{STR} is calculated in the same way as C_{RIV} of the River package, see eq. 3.21.
- **Width of the Stream Channel, Slope of the Stream Channel and Manning's roughness coeff. n/C** are used only when the option **Calculate stream stages in reaches** is checked. The cross-sectional shape of the stream channel is assumed to be rectangular. **Slope of the Stream Channel** is the slope of the stream channel in each reach. **Manning's roughness coeff. n/C** is a value resulting from the Mannings' roughness coefficient n divided by a conversion factor C. Some of the experimental values of the Manning's roughness coefficient can be found in the documentation of the Streamflow-Routing package. The value of the conversion factor C depends on the length and time units of your model.

$$C = 1\ \frac{m^{1/3}}{s} = 1.486\ \frac{ft^{1/3}}{s} = 128383\ \frac{ft^{1/3}}{d} = 86400\ \frac{m^{1/3}}{d} \qquad (3.22)$$

- **Stream Structure** describes the configuration of the stream system. Each row in the table (Fig. 3.23) represents a stream segment in the model. Each segment can have up to 10 tributary segments. The numbers of the tributary segments are specified in the columns 1 to 10. The column **Iupseg** is the number of the upstream segment from which water is diverted. For a segment that is not a diversion, **Iupseg** must be specified as zero. **Iupseg** is used only when the option **Simulate diversions from segments** is checked. The values in Fig. 3.24 indicate that segment 2 is diverted from segment 1, segment 1 is a tributary segment of segment 3, and segments 2 and 4 are tributary segments of segment 5. The configuration of the stream system is shown in Fig. 3.25.

- **Parameter Number** is used to assign the streambed hydraulic conductance C_{STR} as a parameter for an automatic calibration by the inverse models PEST or UCODE, see **PEST ▸ Parameter List...** or **UCODE ▸ Parameter List...**.

Similar to the River package, leakage (Q_1) to or from the aquifer through the streambed is computed by:

$$\begin{aligned} Q_1 &= C_{STR} \cdot (H_s - h) \qquad h > S_{BOT} \\ Q_1 &= C_{STR} \cdot (H_s - S_{BOT}) \qquad h \le S_{BOT} \end{aligned} \tag{3.23}$$

where H_s is the head in the stream, h is the head in the model cell beneath the streambed and S_{BOT} is the elevation of the bottom of the stream.

If the option **Calculate stream stages in reaches** is checked, the depth d in each reach is calculated from Manning's equation under the assumption of a rectangular stream channel:

$$d = \left[\frac{Q \cdot n}{C \cdot w \cdot S^{1/2}} \right]^{3/5} \tag{3.24}$$

where Q [L^3T^{-1}] is the calculated stream discharge, n [-] is Manning's roughness coefficient, w [L] is the width of the channel, S [LL^{-1}] is the slope of the stream channel and C is a conversion factor (see eq. 3.22). Although n and C appear separately here, only the values of n/C or C/n are used in the computer code. You need therefore only to specify the value of n/C in PMWIN.

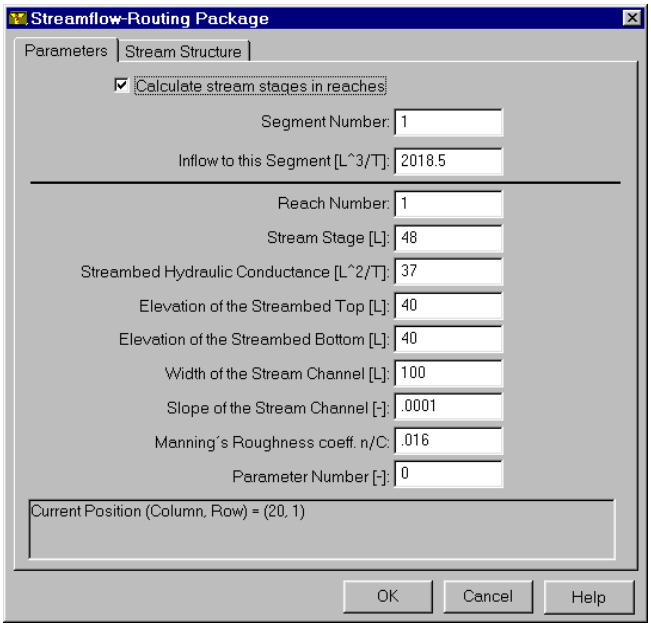
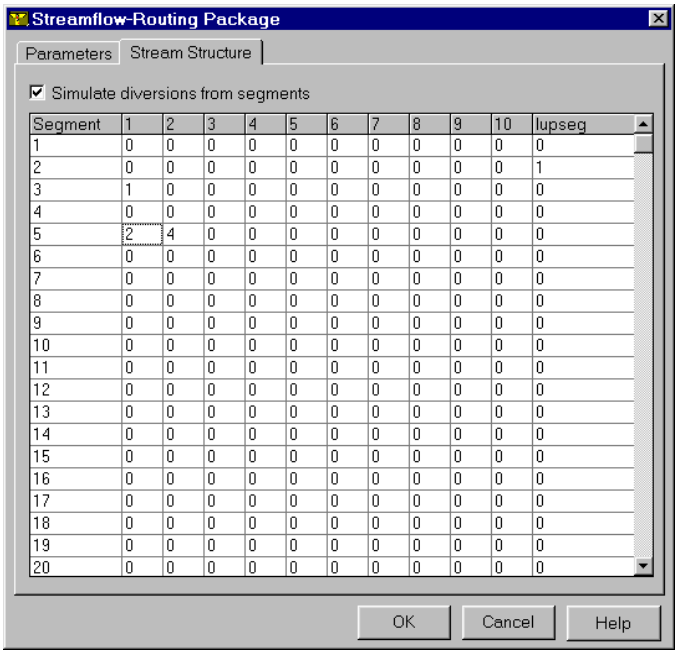


Fig. 3.23 The **Streamflow-Routine Package** dialog box



Segment	1	2	3	4	5	6	7	8	9	10	Iupseg
1	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0	1
3	1	0	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0	0	0
5	2	4	0	0	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0	0	0	0	0
13	0	0	0	0	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0	0	0	0	0
18	0	0	0	0	0	0	0	0	0	0	0
19	0	0	0	0	0	0	0	0	0	0	0
20	0	0	0	0	0	0	0	0	0	0	0

Fig. 3.24 The Stream Structure table of the **Streamflow-Routine Package** dialog box

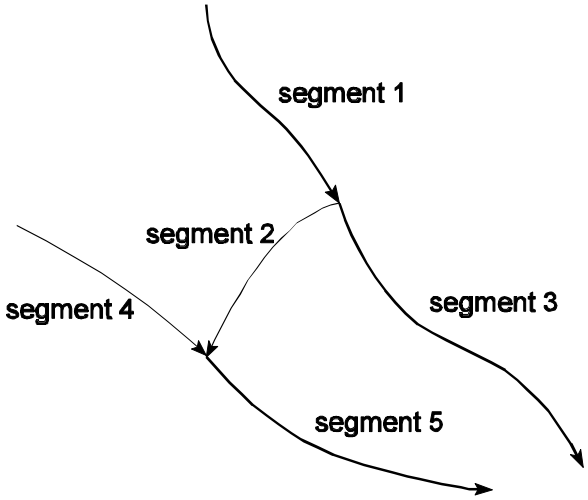


Fig. 3.25 The configuration of the stream system specified in the table of fig. 3.24

MODFLOW ▸ Time-Variant Specified-Head

For transient simulations, the Time-Variant Specified-Head package (Leake and Prudic, 1991) allows fixed-head cells to take on different head values for each time step. The following required data are specified by using the **Time-Variant Specified-Head Package** dialog box (Fig. 3.26) of the **Data Editor**.

- **Flag [-]**. A non-zero value indicates that a cell is specified as a time-variant specified-head boundary.
- **Start Head h_s [L]**. This value is the head in the cell at the start of the stress period.
- **End Head h_e [L]**. This value is the head that will be assigned to the cell for the last time step in the stress period.

This package does not alter the way fixed-head boundaries are formulated in the finite-difference equations of MODFLOW. It simply sets the element in the IBOUND array to a negative value for all cells where a time-variant specified-head boundary is selected (Flag≠0). The package linearly interpolates boundary heads h for each time-variant specified-head boundary cell by using the equation:

$$h = h_s + (h_e - h_s) \cdot \frac{PERTIM}{PERLEN} \qquad (3.25)$$

where PERTIM is the starting time of a time step in a stress period and PERLEN is the length of the stress period. The interpolated heads are constant during a time step. If a cell is specified as a time-variant specified-head boundary for a stress period and omitted in the specification for a subsequent period, it remains a fixed-head boundary with a head equal to that at the end of the previous period.

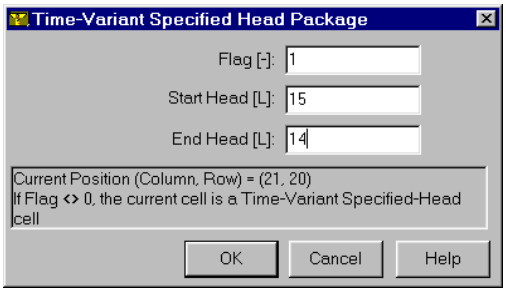


Fig. 3.26 The **Time-Variant Specified-Head Package** dialog box

MODFLOW ▸ Well

An injection or a pumping well is defined by using the **Data Editor** to assign two values to a model cell:

- Rechage rate of the well (Q) [L^3T^{-1}] and
- Parameter Number [-]

Negative cell values for the **"Rechage rate of the well"** are used to indicate pumping wells, while positive cell values indicate injection wells. The parameter number is used to assign Q as a parameter for an automatic calibration by the inverse models PEST or UCODE, see **PEST ▸ Parameter List...** or **UCODE ▸ Parameter List...**.

The injection or pumping rate of a well is constant during a given stress period and is independent of both the cell area and the head in the cell. It is implicitly assumed by MODFLOW that a well penetrates the full thickness of the cell. MODFLOW can simulate wells that penetrate more than one model layer. In this case, the injection or pumping rate for each layer has to be specified. The total injection or pumping rate for a multilayer well is equal to the sum of those from the individual layers. For confined layers, the injection or pumping rate for each layer (Q_k) can be approximately calculated by dividing the total rate (Q_{total}) in proportion to the layer transmissivities (McDonald and Harbaugh, 1988):

$$Q_k = Q_{total} \cdot \frac{T_k}{\Sigma T} \qquad (3.26)$$

where T_k is the transmissivity of layer k and ΣT is the sum of the transmissivities of all layers penetrated by the multilayer well.

Another possibility to simulate a multi-layer well is to set a very large vertical hydraulic conductivity (or vertical leakance), e.g. 1 m/s, to all cells of the well. The total pumping rate is then assigned to the lowest cell of the well. For display purposes, a very small pumping rate (say, -1×10^{-10} m^3/s) can be assigned to other cells of the well. In this way, the exact extraction rate from each penetrated layer will be calculated by MODFLOW implicitly and the value can be obtained by using the **Water Budget Calculator**. See Chapter 2 for how to calculate subregional water budgets.

MODFLOW ▸ Wetting Capability...

The wetting capability of the Block-Centered Flow 2 package (BCF2; McDonald et al. 1991) allows the simulation of a rising water table into unsaturated (dry) model layers.

The BCF2 package is identical to the BCF1 package of the "original" MODFLOW (McDonald and Harbaugh, 1988) except for the wetting and drying of cells. A cell falls dry when the head is below the bottom elevation of the cell. When a cell falls dry, IBOUND is set to 0 (which indicates a no flow or an inactive cell), all conductances to the dry cell are set to zero. No water can flow into the cell as the simulation proceeds and the cell remains inactive even if neighbouring water tables rise again.

To overcome this problem, a value THRESH, called *wetting threshold*, is introduced to the BCF2 package (or later versions of this package). The computer code uses this value to decide, whether a dry or an inactive cell can be turned into a wet (active) cell.

1. If THRESH=0, the dry cell or the inactive cell cannot be wetted.
2. If THRESH<0, only the cell below the dry cell (or inactive cell) can cause the cell to become wet.
3. If THRESH>0, the cell below the dry cell (or inactive cell) and the four horizontally adjacent cells can cause the cell to become wet.

A dry cell or an inactive cell can be turned into an active cell if the head from the previous iteration in a neighboring cell is greater than or equal to the turn-on threshold TURNON.

$$TURNON = BOT + |THRESH| \tag{3.27}$$

where BOT is the elevation of the bottom of the cell.

To keep the stability of the numerical solution, a neighboring cell cannot become wet as a result of a cell that has become wet in the same iteration; only variable-head cells either immediately below or horizontally adjacent to the dry cell can cause the cell to become wet. When a cell is wetted, its IBOUND value is set to 1 (which indicates a variable-head cell), vertical conductances are set to the original values, and the hydraulic head h at the cell is set by using one of the following equation.

$$h = BOT + WETFCT(hn - BOT) \tag{3.28}$$

$$h = BOT + WETFCT \cdot |THRESH| \tag{3.29}$$

where hn is the head at the neighboring cell that causes the dry cell to wet and WETFCT is a user-specified constant called the wetting factor. You may select between eq. 3.28 and 3.29 in the **Wetting Capability** dialog box (Fig. 3.27). This dialog box appears after selecting **MODFLOW▸ Wetting Capability...** from the **Models** menu.

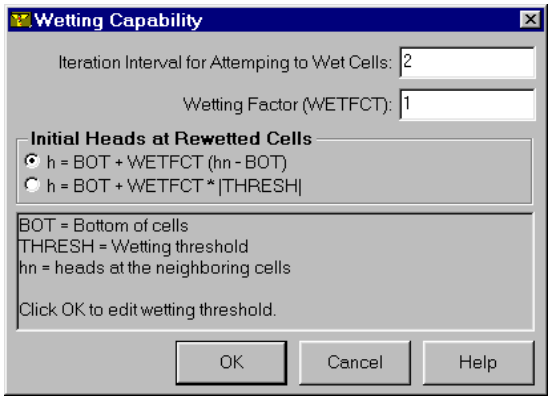


Fig. 3.27 The **Wetting Capability** dialog box

The dialog box also allows you to specify the iteration interval for attempting to wet cells IWETIT. Wetting is attempted every IWETIT iterations. When using the PCG2 solver (Hill, 1990), this applies to outer iterations and not inner iterations. The reason for adjusting IWETIT is that the wetting of cells sometimes produces erroneous head changes in neighboring cells during the succeeding iteration, which may cause erroneous conversions of those cells. These erroneous conversions can be prevented by waiting a few iterations until heads have had a chance to adjust before testing for additional conversions. When setting IWETIT greater than one, there is some risk that cells may be prevented from correctly converting from dry to wet. If the solution for a time step is obtained in less than IWETIT iterations, then there will be no check during that time step to see if cells should be converted from dry to wet. The potential for this problem to occur is greater in transient simulations, which frequently require only a few iterations for a time step.

The method of wetting and drying cells used in the BCF2 Package can cause problems with the convergence of the iterative solvers used in MODFLOW. Convergence problems can occur in MODFLOW even without the wetting capability but problems are more likely to occur when the wetting capability is used. Symptoms of a problem are slow convergence or divergence combined with the frequent wetting and drying of the same cells. It is normal for the same cell to convert between wet and dry several times during the convergence process but frequent conversions are an indication of problems. As a matter of fact, situations exist where the real solution oscillates such as in the case of a well causing a drawdown which makes the well cells fall dry. This in turn switches off the well and leads to a rise of the water table and wetting of the well cell etc. The user can detect such situations by examining the model run record file

OUTPUT.DAT; a message is printed each time a cell converts. Refer to the documentation of the BCF2 package for how to solve problems with convergence.

MODFLOW ▸ Output Control

The **Output Control** menu is used to control the frequency and terms of simulation results of MODFLOW that will be printed or saved. Various simulation results can be saved in files by checking the corresponding output terms in the **MODFLOW Output Control** dialog box (Fig. 3.28). The simulation results are saved whenever the time steps and stress periods are an even multiple of the **output frequency** and the results for the first and last stress periods and time steps are always saved. Use 0 (zero) for the output frequency, if only the result of the last stress period or the last time step should be saved. The predefined heads for no-flow cells (HNOFLO) and dry cells (HDRY) are given in the **Predefined Head Values** group.
The output terms and the corresponding result files are described below. All result files are saved in the folder in which your model data are saved.

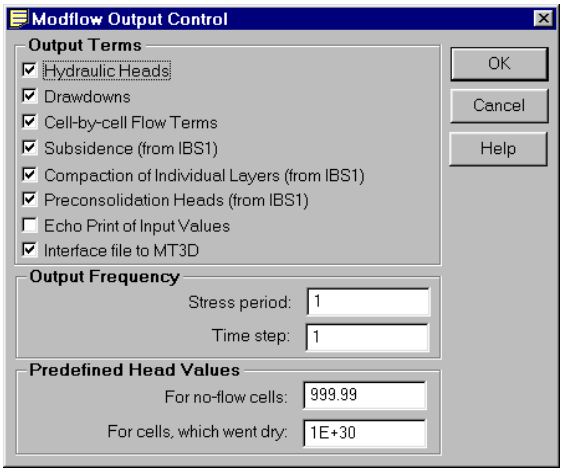


Fig. 3.28 The **MODFLOW Output Control** dialog box

- **Hydraulic Heads** are the primary result of a MODFLOW simulation. Hydraulic heads in each finite-difference cell are saved in the unformatted (binary) file HEADS.DAT.
- **Drawdowns** are the differences between the initial hydraulic heads and the calculated hydraulic heads. Drawdowns in each cell are saved in the unformatted (binary) file DDOWN.DAT.
- **Cell-by-cell Flow Terms** are flow terms for individual cells, including four types: (1) cell-by-cell stress flows, or flows into or from an individual cell due to one of the external stresses (excitations) represented in the model, e.g., pumping well or recharge; (2) cell-by-cell storage

terms, which give the rate of accumulation or depletion of storage in an individual cell; (3) cell-by-cell constant-head flow terms, which give the net flow to or from individual constant-head cells; and (4) internal cell-by-cell flows, which are the flows across individual cell faces, that is, between adjacent model cells. The cell-by-cell flow terms are used for calculating water budgets and for particle tracking and transport simulations by *PMPATH* and MOC3D. The cell-by-cell flow terms are saved in the unformatted (binary) file BUDGET.DAT.

- **Subsidence** is the sum of the compaction of all model layers, for which the interbed strorage calculation is turned on (see Layer Type in section 3.4).
- **Compaction of individual layers** is the sum of the calculated compaction and the user-specified starting compaction in each layer.
- **Preconsolidation head** is the previous minimum head value in the aquifer. For model cells in which the specified preconsolidation head is greater than the corresponding value of starting head, the preconsolidation head will be set to the starting head. Subsidence, compaction and preconsolidation head are saved in the unformatted (binary) file INTERBED.DAT.
- **Interface file to MT3D** is an unformatted (binary) file containing the computed heads, fluxes across cell interfaces in all directions and locations and flow rates of the various sinks/sources. The interface file is created by the LKMT package provided by MT3D or MT3DMS. There are three versions of the LKMT package, which are incorporated in the versions of MODFLOW contained in the PMWIN (see **MODFLOW ▸ Run...** below). The LKMT1 package creates interface file to the version 1.xx of MT3D. The LKMT2 package creates interface file to MT3D96 and MT3D_Dod_1.5. The LKMT3 package creates interface file to MT3DMS.

To check the simulation results, MODFLOW calculates a volumetric water budget for the entire model at the end of each time step, and saves the results in the simulation record file OUTPUT.DAT. A water budget provides an indication of the overall acceptability of the numerical solution. In numerical solution techniques, the system of equations solved by a model actually consists of a flow continuity statement for each model cell. Continuity should therefore also exist for the total flows into and out of the entire model or a sub-region. This means that the difference between total inflow and total outflow should equal the total change in storage. It is recommended to read the record file. The record file also contains other essential information. In case of difficulties, this supplementary information could be very helpful.

MODFLOW ▸ Solvers

To calculate heads in each cell in the finite-difference grid, MODFLOW prepares one finite difference equation for each cell, expressing the relationship between the head at a node and the heads at each of the six adjacent nodes at the end of a time step. Because each equation may involve up to seven unknown values of head, and because the set of unknown head values changes from one equation to the next through the grid, the equations for the entire grid must be solved simultaneously at each time step. The system of simultaneous finite difference linear equations can be expressed in matrix notation as

$$\underline{A} \cdot \underline{x} = \underline{b} \qquad (3.30)$$

where $\underline{A}$ is a coefficient matrix assembled by MODFLOW using user-specified model data; $\underline{b}$ is a vector of defined flows, terms associated with head-dependent boundary conditions and storage terms at each cell; $\underline{x}$ is a vector of hydraulic heads at each cell. One value of the hydraulic head for each cell is computed at the end of each time step. At present PMWIN supports four packages (solvers) for solving systems of simultaneous linear equations:

- the Direct Solution (DE45) package,
- the Preconditioned Conjugate-Gradient 2 (PCG2) package,
- the Strongly Implicit Procedure (SIP) package, and
- the Slice-Successive Overrelaxation(SSOR) package.

Input parameters of these solution methods are discussed below. See McDonald and Harbaugh (1988), Hill (1990a) and Harbaugh (1995) for detailed mathematical background and numerical implementation of these solvers. Various comparisons between the solution methods can be found in Trescott (1977), Behie and Forsyth (1983), Scandrett (1989) and Hill (1990b). Hill indicates that the greatest differences in solver efficiency on scalar computers occur for three-dimensional, non-linear problems. For these types of problems, it may be well worth the time and effort to try more than one solver. If your model does not have a large number of active cells, you may try to use the direct solver (DE45). Otherwise, SIP generally is a good alternative to consider.Note that the MODFLOW version “MODFLOW + Density package from KIWA” does not support the Direction Solution package.

MODFLOW ▸ Solvers ▸ DE45...

Although a direct solver requires more memory and typically requires more computational effort than iterative solvers, it may excute faster than an iterative solver in some situations. The Direct Solution package (Harbaugh, 1995) uses Gaussian elimination with an alternating diagonal equation numbering scheme that is more efficient than the standard method of equation numbering. It is the most efficient when solving small, linear problems.

Use the **Direct Solution (DE45)** dialog box (Fig. 3.29) to specify required parameters as described below:

- **Max. iterations (external or internal)** is the maximum number of iterations in each time step. Set this number to 1 if iteration is not desired. Ideally iteration would not be required for direct solution; however, it is necessary to iterate if the flow equation is non-linear (see Problem type below) or if computer precision limitations result in inaccurate calculations as indicated by large water budget error. For a non-linear flow equation, each iteration is equally time consuming because the coefficient matrix $\underline{A}$ is changed each iteration and Gaussian elimination is required after each change. This is called external iteration. For a linear equation, iteration is significantly faster because $\underline{A}$ is changed at most once per time step; thus, Gaussian elimination is required at most once per time step. This is called internal iteration.
- **Max. equations in upper part of [A]**: This is the maximum number of equations in the upper part of the equations to be solved. This value impacts the amount of memory used by the solver. If specified as 0, the program will calculate the value as half the number of cells in the model, which is an upper limit. The actual number of equations in the upper part will be less than half the number of cells whenever there are no-flow and constant head cells because flow equations are not formulated for these cells. The solver prints the actual number of equations in the upper part when it runs. The printed value can be used in future runs in order to minimize memory usage.
- **Max. equations in lower part of [A]**: This is the maximum number of equations in the lower part of the equations to be solved. This value impacts the amount of memory used by the solver. If specified as 0, the program will calculate the value as half the number of cells in the model, which is an upper limit. The actual number of equations in the lower part will be less than half the number of cells whenever there are no-flow and constant head cells because flow equations are not formulated for these cells. The solver prints the actual number of equations in the lower part when it runs. The printed value can be used in future runs in order to minimize memory usage.

- **Max. band width of AL**: This value impacts the amount of memory used by the solver. If specified as 0, the program will calculate the value as the product of the two smallest grid dimensions, which is an upper limit.
- **Head change closure criterion [L]**: If iterating, iteration stops when the absolute value of head change at every node is less than or equal to this value. The criterion is not used when not iterating, but a value must always be specified.

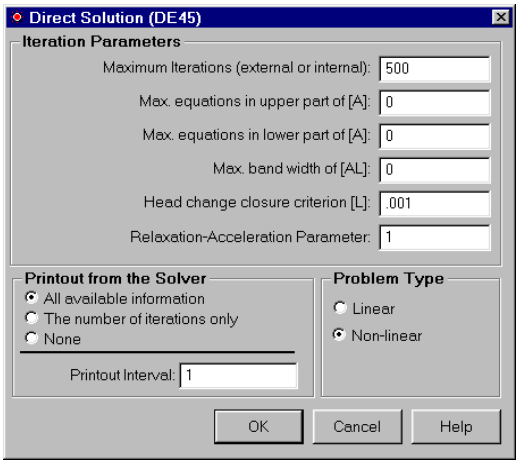


Fig. 3.29 The **Direct Solution (DE45)** dialog box

- **Printout From the Solver**: If the option **All available information** is selected, the maximum head change and residual (positive or negative) are saved in the run record file OUTPUT.DAT for each iteration of a time step whenever the time step is an even multiple of **Printout Interval**. If the option **The number of iterations only** is checked, the printout of maximum head change and residual is suppressed. Select the option **None** to suppress all printout from the solver. A positive integer is required by **Printout Interval**.
- **Problem Type**: The choice of problem type affects the efficiency of solution; significant work can be avoided if it is known that A remains constant all or part of the time.

  Linear indicates that the flow equations are linear. To meet the linearity requirement, all model layers must be confined, and there must be no formulations that change based upon head (such as seepage from a river changing from head dependent flow to a constant flow when head drops below the bottom of the riverbed). Examples of non-linearity are cases with riverbed conductance, drain conductance, maximum evapotranspiration rate, evapotranspiration extinction depth, gerneral-head boundary conductance and reservior-bed conductance.

  Nonlinear indicates that a non-linear flow equation is being solved, which means that some terms in A depend on simulated head. Example of head-dependent terms in A are

transmissivity for water-table layers, which is based on the saturated thickness; flow terms for rivers, drains, and evapotranspiration of they convert between head dependent flow and constant flow; and the change in storage coefficient when a cell converts between confined and unconfined. When a non-linear flow equation is being solved, external iteration is normally required in order to accurately approximate the non linearities. Note that when non linearities caused by water-table calculations are part of a simulation, there are not necessarily any obvious signs in the output from a simulation that does not use external iteration to indicate that iteration is needed. In particular, the budget error may be acceptably small without iteration even though there is significant error in head because of non linearity. To understand this, consider the water-table correction for transmissivity. Each iteration a new transmissivity is calculated based on the previous head. Then the flow equations are solved, and a budget is computed using the new head with the same transmissivities. No budget discrepancy results becuase heads are correct for the transmissivity being used at this point; however, the new heads may cause a significant change in transmissivity. The new transmissivity will not be calculated unless there is another iteration. Therefore, when one or more layers is under water-table conditions, iteration should always be tried. The maximum change in head during each iteration (printed by the solver) provides an indication of the impact of all non linearities.

MODFLOW ▸ Solvers ▸ PCG2...

The required parameters for the PCG2 package are specified in the **Preconditioned Conjugate-Gradient Package 2** dialog box (Fig. 3.30). They are described below:

- **Preconditioning Method:** The PCG2 package provides two preconditioning options: the **modified incomplete Cholesky preconditioner** MICCG (Axelsson and Lindskog, 1986) and the **Neuman Series Polynomial preconditioner** POLCG (Saad, 1985).
- **Relaxation Parameter** is used with MICCG. Usually, this parameter is equal to 1. Ashcraft and Grimes (1988) found out that for some problems a value of 0.99, 0.98 or 0.97 will reduce the number of iterations required for convergence.
- The option **Calculate the upper bound on the maximum eigenvalue** is only available when POLCG is selected. Check this box, if the upper bound on the maximum eigenvalue of A should be calculated by the solver. Otherwise, a value of 2 will be used. The upper bound is estimated as the largest sum of the absolute values of the components in any row of A. Convergence is generally insensitive to this value. Estimation of the upper bound uses slightly more execution time per iteration.

- **Allowed Iteration Numbers: MXITER** is the maximum number of outer iterations. For each outer iteration, $\underline{A}$ and $\underline{b}$ (eq. 3.30) are updated by using the newly calculated hydraulic heads. For a linear problem, MXITER should be 1, unless more that 50 inner iterations are required. A larger number (generally less than 100) is required for a nonlinear problem. Outer interations continue until the final convergence criteria (see below) are met on the first inner iteration. **ITER1** is the maximum number of inner iterations. Eq. 3.30 with a new set of $\underline{A}$ and $\underline{b}$ is solved in inner iterations. The inner iterations continue until ITER1- iterations are executed or the final convergence criteria (see below) are met.
- **Convergence Criteria: Head Change [L]** is the head change criterion for convergence. When the maximum absolute value of the head change at all nodes during an iteration is less than or equal to the specified Head Change, and the criterion for Residual is satisfied (see below), iteration stops. **Residual [L^3T^{-1}]** is the residual criterion for convergence. Residual is calculated as $\underline{b} - \underline{A} \cdot \underline{x}$ for each inner iteration. When the maximum absolute value of the residual at all cells during an iteration is less than or equal to Residual, and the criterion for Head Change is satisfied (see above), iteration stops.
- **Printout From the Solver**: A positive integer is required by Printout Interval. If the option **All available information** is selected, the maximum head change and residual (positive or negative) are saved in the run record file OUTPUT.DAT for each iteration of a time step whenever the time step is an even multiple of Printout Interval. If the option **The number of iterations only** is checked, the printout of maximum head change and residual is suppressed. Select the option **None** to suppress all printout from the solver.

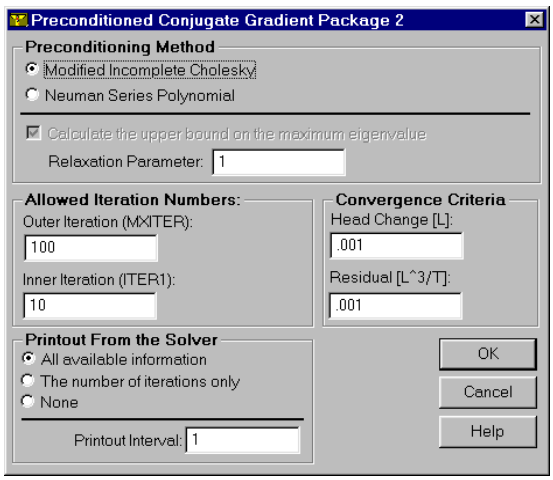


Fig. 3.30 The **Preconditioned Conjugate Gradient Package 2** dialog box

MODFLOW ▸ Solvers ▸ SIP

The required parameters for the SIP package are specified in the **Strongly Implicit Procedure Package** dialog box (Fig. 3.31). The parameters are described below:

- **MXITER** is the maximum number of iterations in one time step in an attempt to solve the system of finite-difference equations.
- **IPRSIP** is the printout interval for this package. A positive integer is required. The maximum head change (positive or negative) is saved in the run record file OUTPUT.DAT for each iteration of a time step whenever the time step is an even multiple of IPRSIP. This printout also occurs at the end of each stress period regardless of the value of IPRSIP.
- **NPARM** is the number of iteration parameters to be used. Five parameters are generally sufficient.
- **ACCL** is the acceleration parameter. It must be greater than zero and is generally equal to one.
- **Head Change [L]** is the head change criterion for convergence. When the maximum absolute value of head change from all cells during an iteration is less than or equal to Head Change, iteration stops.

MODFLOW ▸ Solvers ▸ SSOR

The required parameters for SSOR package are specified in the **Slice Successive Overrelaxation Package** dialog box (Fig. 3.32). The parameters are described below:

- **MXITER** is the maximum number of iterations in one time step in an attempt to solve the system of finite-difference equations.
- **IPRSOR** is the printout interval for SSOR. A positive integer is required. The maximum head change (positive or negative) is saved in the run record file OUTPUT.DAT for each iteration of a time step whenever the time step is an even multiple of IPRSOR. This printout also occurs at the end of each stress period regardless of the value of IPRSOR.
- **ACCL** is the acceleration parameter, usually between 1.0 and 2.0.
- **Head Change** is the head change criterion for convergence. When the maximum absolute value of head change from all cells during an iteration is less than or equal to Head Change, iteration stops.

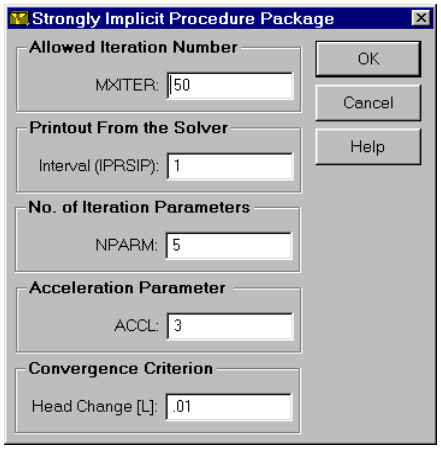


Fig. 3.31 The **Strongly Implicit Procedure Package** dialog box

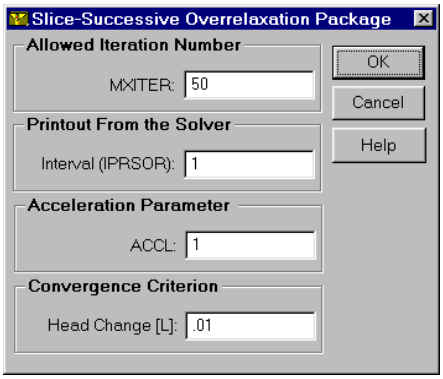


Fig. 3.32 The **Slice Successive Overrelaxation Package** dialog box

MODFLOW ▸ Run...

Select this menu item, if you want to check the model data or run the flow simulation with MODFLOW. The available settings of the **Run Modflow** dialog box (Fig. 3.33) are described below.

- **Modflow Version** and **Modflow Program:** Several variants of MODFLOW are included in PMWIN, all of them are compiled with a FORTRAN compiler of Lahey. PMWIN automatically installs the executables of these variants. Their full paths and file names are given in table 3.4. If you want to use a compiled version located in another position, click the **open file** button  and select the desired code from a dialog box. The **User's own** version must be selected, if you want to use your own version of MODFLOW. Refer to Appendix 5 for how to configure PMWIN to run with your own MODFLOW.
- **The File Table:** PMWIN uses the user-specified data to generate input files for MODFLOW

and MODPATH. **Description** gives the name of the packages used in the flow model. The path and name of the input file are shown in **Destination File**. PMWIN generates an input file only if the corresponding **Generate** flag is checked. You may click on a flag to check or uncheck it. Normally, you do not need to worry about these flags, as PMWIN will take care of the settings. Note that you cannot run MODPATH (Pollock, 1989) and/or MODPATH-PLOT (Pollock, 1994) from PMWIN directly. See Appendix 6 for how to run these programs.

- **Options**:
  - **Regenerate all input files for MODFLOW:** You should check this option, if the input files have been deleted or overwritten by other programs.
  - **Check the model data:** Before creating data files for MODFLOW, PMWIN will check the geometry of the model and the consistency of the model data as given in table 3.5, if this option is checked. The errors (if any) are saved in the file CHECK.LST located in the same folder as your model data.
  - **Generate input files only, don't start MODFLOW:** Check this option, if you do not want to run MODFLOW. You can start the simulation at a later time by executing the batch file MODFLOW.BAT.
- **OK**: Click **OK** to start the generation of MODFLOW input files. In addition, PMWIN generates a batch file MODFLOW.BAT saved in your model folder. When all necessary files are generated, PMWIN automatically runs MODFLOW.BAT in a DOS-window. During a flow simulation, MODFLOW writes a detailed run record to the file OUTPUT.DAT saved in your model folder. MODFLOW saves the simulation results in various unformatted (binary) files only if a flow simulation has been successfully completed. See **MODFLOW ▸ Output Control** for details about the output terms from MODFLOW.

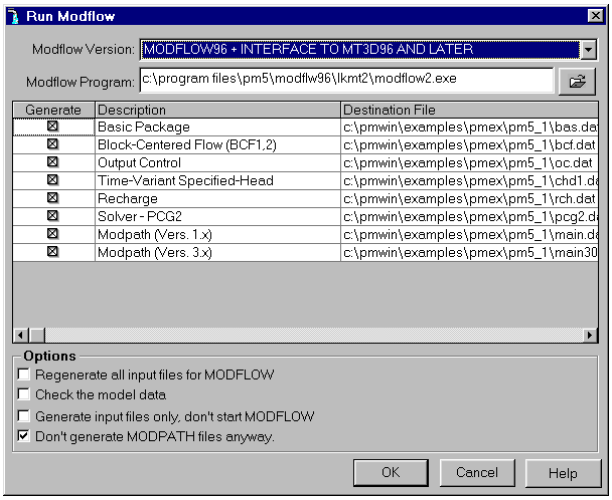


Fig. 3.33 The **Run Modflow** dialog box

Table 3.4 Versions and filenames of MODFLOW

Version	Filename
MODFLOW96	*pmhome*\modflw96\usgs\modflw96.exe
MODFLOW96+INTERFACE TO MT3D 1.XX	*pmhome*\modflw96\lkmt1\modflow1.exe
MODFLOW96+INTERFACE TO MT3D96	*pmhome*\modflw96\lkmt2\modflow2.exe
MODFLOW+INTERFACE TO MT3DMS	*pmhome*\mt3dms\modf.exe
MODFLOW+DENSITY PACKAGE FROM KIWA	*pmhome*\modflow\density\modden.exe
PMWIN 4.X (+ interface to MT3D 1.XX)	*pmhome*\modflow\lkmt1\mflowpm4.exe
PMWIN 4.X (+ interface to MT3D96)	*pmhome*\modflow\lkmt2\mflowpm4.exe

- *pmhome* is the folder in which PMWIN is installed, for example C:\Program Files\PM5.
- **The memory allocation of the so-called "X-array" is fixed in MODFLOW96. This means the maximum number of cells is limited at a certain level when you use MODFLOW96. Use the versions of PMWIN 4.X, if you have a large model.**
- Note that the corresponding source code of these programs (except the density package) can be found in the Source folder of the distribution CD.

Table 3.5 Model data checked by PMWIN

Term	Checking Criteria
layer thickness	may not be zero or negative
top and bottom elevation of layers	consistency of the elevations
initial head at fixed-head cells	a fixed-head cell may not be dry at the beginning of a simulation.
Horizontal hydraulic conductivity, transmissivity, vertical hydraulic conductivity, vertical leakance or effective porosity	may not be zero or negative
Storage coefficient, specific storage, or specific yield	may not be negative
River package	1. a river cell may not be a fixed-head cell and should not be an inactive cell. 2. elevation of the riverbed should be higher than the elevation of the cell bottom. 3. the river stage must be higher than elevation of the riverbed.
Drain package	1. a drain cell may not be a fixed-head cell and should not be an inactive cell. 2. elevation of the drain should be higher than the elevation of the cell bottom
General-head boundary	a GHB-cell may not be a fixed-head cell and should not be an inactive cell.
Streamflow-Routing package	a STR-cell may not be a fixed-head cell and should not be an inactive cell.
Well package	a well-cell may not be a fixed-head cell and should not be an inactive cell

3.6.2 MOC3D

MOC3D ▸ Subgrid...

Within the finite-difference grid used to solve the flow equation in MODFLOW, the user may specify a window or subgrid over which MOC3D will solve the solute-transport equation. This feature can significantly enhance the overall efficiency of the model by avoiding calculation effort where it is not needed. However, MOC3D requires that within the area of the transport subgrid, row and column discretization must be uniformly spaced (that is, Δx and Δy must be constant, although they need not be equal to each other). The spatial discretization or rows and columns beyond the boundaries of the subgrid can be nonuniform, as allowed by MODFLOW, to permit calculations of head over a much larger area than the area of interest for transport simulation. Vertical discretization, defined by the cell thickness, can be variable in all three dimensions. However, large variability may adversely affect numerical accuracy. For details, refer to Konikow et al. (1996) for the model assumptions that have been incorporated into the MOC3D model.

The subgrid is defined in the **Subgrid for Transport (MOC3D)** dialog box (Fig. 3.34). MOC3D assumes that the concentration outside of the subgrid is the same within each layer, so only one concentration value is specified for each layer within or adjacent to the subgrid by using the **C' Outside of Subgrid** table of this dialog box. The values of other layers, which are not within or adjacent to the subgrid, are ignored.

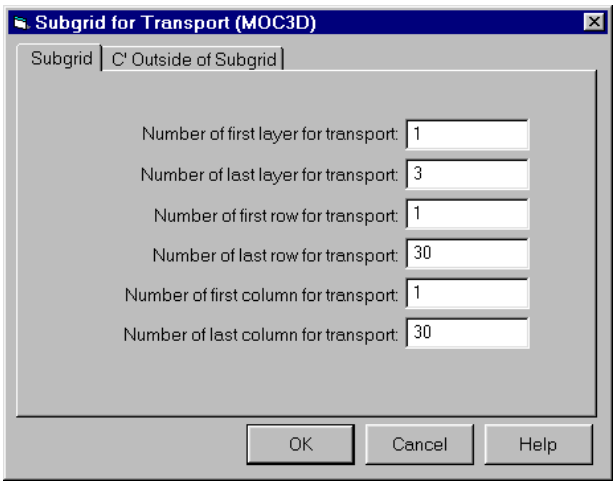


Fig. 3.34 The **Subgrid for Transport (MOC3D)** dialog box

MOC3D ▸ Initial Concentration

MOC3D requires initial concentration of each cell within the transport subgrid at the beginning of a transport simulation. The values specified here are shared with MT3D.

MOC3D ▸ Advection...

Use the **Parameter for Advective Transport (MOC3D)** dialog box (Fig. 3.35) to specify the required data as described below.

- **Interpolation scheme for particle velocity:** In MOC3D, the advection term of a solute transport process is simulated by the Method of Characteristics (MOC). Using the MOC scheme, a set of moving particles is distributed in the flow field at the beginning of the simulation. A concentration and a position in the Cartesian coordinate system are associated with each of these particles. Particles are tracked forward through the flow field using a small time increment. At the end of each time increment, the average concentration at a cell due to advection alone is evaluated from the concentrations of particles which happen to be located within the cell. The other terms in the governing equation, i.e. dispersion, chemical reaction and decay, are accounted for by adjusting the concentrations associated with each particle.

  A moving particle in a ground-water flow system will change velocity as it moves due to both spatial variation in velocity and temporal variations during transient flow. During a flow time step, advection is determined from velocities computed at the end of the flow time step. Temporal changes in velocity are accounted for by a step change in velocity at the start of each new flow time step. After the flow equation is solved for a new time step, the specific discharge across every face of each finite-difference cell is recomputed on the basis of the new head distribution, and the movement of particles during this flow time step is based only on these specific discharges.

  MOC3D provides two interpolation options - linear and bilinear interpolation, for calculating the spatial variation of the particle velocity from the specific discharges. Konikow et al. (1996) indicate that if transmissivity within a layer is homogeneous or smoothly varying, bilinear interpolation of velocity yields more realistic pathlines for a given discretization than linear interpolation. And, in the presence of strong heterogeneities between adjacent cells within a layer, it would usually be preferable to select the linear interpolation scheme.
- **Maximum number of particles** (NPMAX): Maximum number of particles available for particle tracking of advective transport in MOC3D. If set to zero, the model will calculate

NPMAX according to eq. 3.31.

$$NPMAX = 2 \cdot NPTPND \cdot NSROW \cdot NSCOL \cdot NSLAY \quad (3.31)$$

where NPTPND is the initial number of particles per cell (see below). The values NSROW, NSCOL and NSLAY are the number of rows, columns and layers of the transport subgrid, respectively.

- **Courant number** (CELDIS) is the number of cells (or the fraction of a cell) that a particle may move through in one step (typically, $0.5 \leq$ CELDIS ≤ 1.0).
- **Fraction limit for regenerating initial particles** (FZERO): If the fraction of active cells having no particles exceeds FZERO, the program will automatically regenerate an initial particle distribution before continuing the simulation (typically, $0.01 \leq$ FZERO ≤ 0.05).
- **Initial number of particles per cell** (NPTPND): Valid options for default geometry of particle placement include 1, 2, 3, or 4 for one-dimensional transport simulation; 1, 4, 9, or 16 for two-dimensional transport simulation; and 1, 8, or 27 for three-dimensional transport simulation. The user can also customize initial placement of particles by specifying a negative number to NPTPND, pressing the **Tab**-key and entering local particle coordinates into table in the lower part of the dialog box shown in Fig. 3.35, where PNEWL, PNEWR and PNEWC are relative positions for the initial placement of particles in the layer, row and column direction, respectively. The local coordinate system range is from -0.5 to 0.5, and represents the relative distance within the cell about the node location at the center of the cell, so that the node is located at 0.0 in each direction.

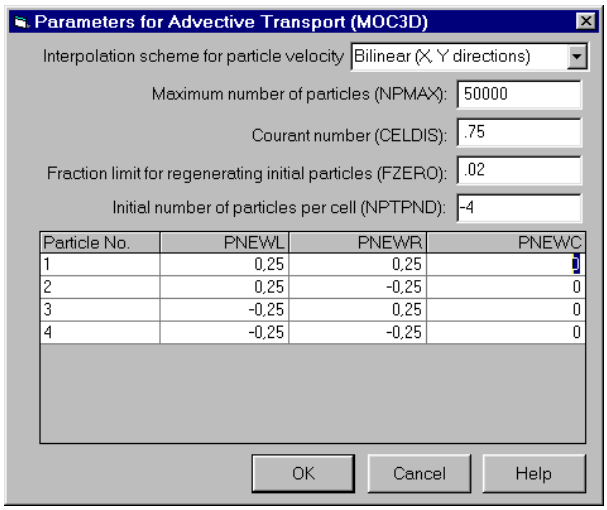


Fig. 3.35 The **Parameters for Advective Transport (MOC3D)** dialog box

MOC3D ▸ Dispersion & Chemical Reaction...

The types of reactions incorporated into MOC3D are restricted to those that can be represented by a first-order rate reaction, such as radioactive decay, or by a retardation factor, such as instantaneous, reversible, sorption-desorption reactions governed by a linear isotherm and constant distribution coefficient (K_d).

Use the **Dispersion / Chemical Reaction (MOC3D)** dialog box (Fig. 3.36) to specify the required data for each model layer as described below.

- **Simulate Dispersion**: Check this option, if dispersion should be included in the simulation.
- **First order decay rate** λ [T^{-1}] typically represents represents radioactive decay of both the free and sorbed solute. A radioactive decay rate is usually expressed as a half-life ($t_{1/2}$). The half-life is the time required for the concentration to decrease to one-half of the original value. λ is calculted by:

$$\lambda = \frac{\ln 2}{t_{1/2}} \tag{3.32}$$

- **Effective molecular diffusion coefficient** [L^2T^{-1}] describes the diffusive flux of a solute in water from an area of greater concentration toward an area where it is less concentrated. The mass flux is proportional to the concentration gradient and is given by Fick's first law:

$$F = -D \cdot \frac{dC}{dx} \tag{3.33}$$

where F [$ML^{-2}T^{-1}$] is the mass flux of solute per unit area per unit time; D [L^2T^{-1}] is the diffusion coefficient; C [ML^{-3}] is the solute concentration and dC/dx [$ML^{-3}L^{-1}$] is the concentration gradient. In porous media, the solute mass cannot diffuse as fast as in free water, because the ions must move along longer pathways through the pore space and because of adsorption on the soil matrix. To account for this tortuosity effect, an effective diffusion coefficient D^* must be used.

$$D^* = \omega \cdot D \tag{3.34}$$

According to Freeze and Cherry (1979), ω ranges from 0.5 to 0.01 for laboratory studies of diffusion of nonadsorbed ions in porous geologic materials. The diffusion coefficients D of the major ions (Na^+, K^+, Mg^{2+}, Ca^{2+}, Cl^-, CO_3^{2-} HCO_3^-, SO_4^{2-}) are temperature-dependent and range from 1×10^{-9} to 2×10^{-9} m^2/s at 25 °C (Li and Gregory, 1974; Robinson and Stokes, 1965). At 5°C the coefficients are about 50% smaller. The molecular diffusion coefficient is

generally very small and negligible compared to the mechanical dispersion (see below) and is only important when groundwater velocity is very low.

- **Longitudinal dispersivity α_L [L], horizontal transverse dispersivity α_{TH} [L] and vertical transverse dispersivity α_{TV} [L]** describe the spreading of the solute concentration in groundwater caused by the irregular shape of the interconnected pore space and the velocity variations at the microscopic level. The velocity of groundwater varies according to the size of the pores and water moves faster at the internal points between soil grains than on the solid surface. This spreading is often referred to as *mechnical dispersion* and it occurs in all three spatial directions. The coefficient of mechanical dispersion is defined by $\alpha_i \cdot v_i$, where α_i is the dispersivity and v_i is the average linear velocity in the i direction. The sum of mechanical dispersion and molecular diffusion is called *hydrodynamic dispersion.*

  Values of dispersivity used for simulations generally depend on the scale of a concentration plume being considered. While a plume "grows", it will not only undergo the microscopic mechnical dispersion but also the dispersion caused by macroscopic heterogeneities. This results to a trend of increasing dispersivity values with the scale of observation. Summaries of the scale-dependent dispersivity values are provided by Anderson (1979, 1984), Gelhar et al. (1985, 1992) and Spitz and Moreno (1996). Note that all heterogeneity which is not explicitly represented in the model has to be incorporated into the dispersion coefficients.
- **Retardation factor** [-]: For a linear isotherm the retardation factor R is independent of the concentration field. R is calculated by

$$R = 1 + \frac{\rho_b}{n} \cdot K_d \qquad (3.35)$$

where n is the porosity of the porous medium.

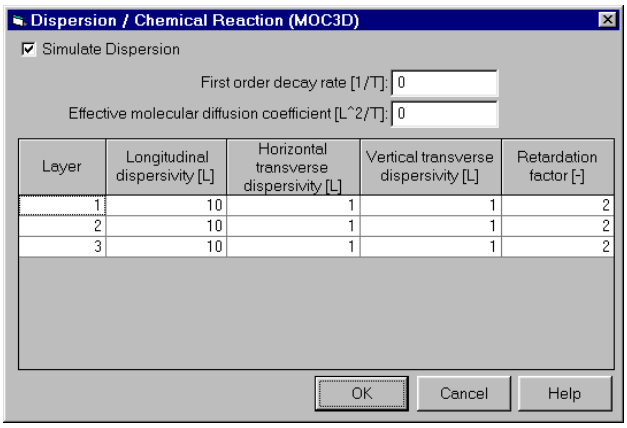


Fig. 3.36 The **Dispersion / Chemical Reaction (MOC3D)** dialog box

MOC3D ▸ Strong/Weak Flag

A flag is required for each cell within the transport subgrid. Where fluid **source** is strong, new particles are added to replace old particles as they are advected out of that cell. Where a fluid **sink** is strong, particles are removed after they enter that cell and their effect has been accounted for. Where sources or sinks are weak, particles are neither added nor removed, and the source/sink effects are incorporated directly into appropriate changes in particle positions and concentrations. **A strong source or sink cell is indicated by the cell value of 1.**

MOC3D ▸ Observation Wells

Cells of the transport subgrid can be designated as **observation wells** by assigning the value of 1 to the cells. At each **observation well**, the time, head, and concentration after each particle move will be written to the separate output file MOCOBS.OUT saved in the same folder as your model data. Note that this feature is to facilitate graphical postprocessing of the calculated data using other software packages outside of PMWIN.

MOC3D ▸ Sink/Source Concentration

This menu is used for specifying the concentrations of point or areally-distributed sources, including fixed-head cells, general-head boundary cells, rivers, wells and recharge cells. Except the concentrations associated with fixed-head cells, all source concentrations are specified by using the **Data Editor**. If the concentration of a fluid source is not specified, the default value for the concentration is zero. The source concentration associated with the fixed-head cells are specified in the **Source Concentration (Fixed-Head)** dialog box (Fig. 3.37). The fixed-head cells are grouped into zones, which are defined by specifying unique negative values to the IBOUND array (see section 3.4). Each zone has an associated source concentration.

The concentration in the fluid leaving the aquifer at fluid sinks is assumed to have the same concentration as the fluid in the aquifer. However, if the fluid sink is associated with evaporation or transpiration, it is assumed that the fluid discharge mechanism will exclude dissolved chemicals, which results in an increase in concentration at the location of the sink.

Items of this menu are dimmed if the corresponding hydraulic features given in the **Models▸Modflow** menu are not used (checked). The specified concentration will be used by MOC3D if a corresponding menu item is checked. If a checked item is no longer necessary for a transport simulation, simply select the item again and deactivate it.

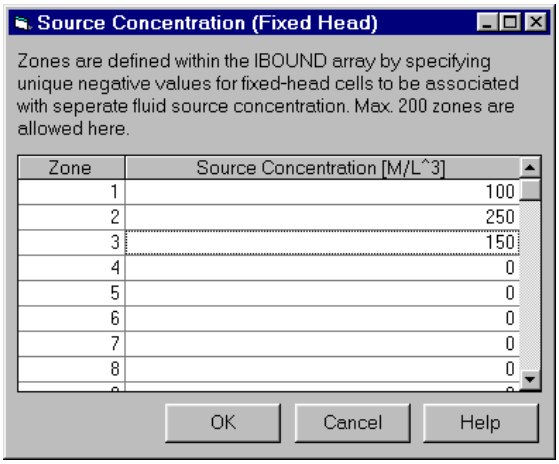


Fig. 3.37 The **Source Concentration (Fixed Head)** dialog box

MOC3D ▸ Output Control...

The main output file of MOC3D is the listing file MOC3D.LST. MOC3D includes output options to create separate ASCII or binary files for concentration, velocity and the location of particles. Optionally the *dispersion equation coefficients* on cell faces can be written to the listing file. The dispersion equation coefficient is a combination of dispersion coefficient D, porosity n, thickness b and an appropriate grid dimension factor. For example, the dispersion equation coefficient for the j+1/2, i, k face in the column direction is $(n \cdot b \cdot D_{xx})_{j+1/2,\,i,\,k} / \Delta x$.

The output from MOC3D is controlled by using the **Output Control (MOC3D)** dialog box (Fig. 3.38). Most items in this dialog box are self-explanatory. The names of the separate ASCII or binary output files are given in Table 3.6.

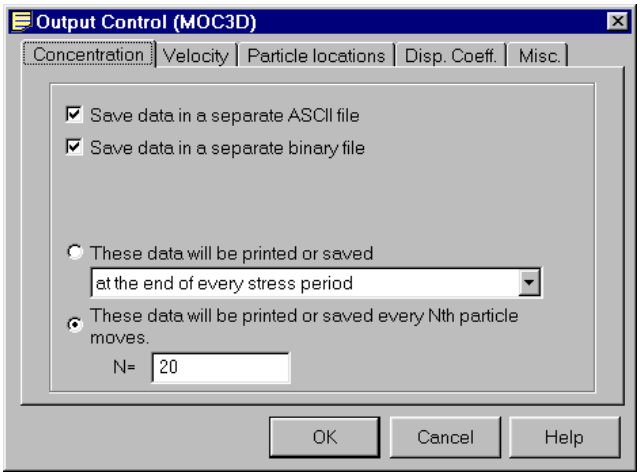


Fig. 3.38 The **Output Control (MOC3D)** dialog box

Table 3.6 Names of the MOC3D output files.

Output Term	Filename
Listing file	*path*\moc3d.lst
Concentration file (ASCII)	*path*\mocconc.asc
Concentration file (binary)	*path*\mocconc.bin
Velocity (ASCII)	*path*\mocvel.asc
Velocity (binary)	*path*\mocvel.bin
particle location (ASCII)	*path*\mocprt.asc
particle location (binary)	*path*\mocprt.bin

- *path* is the folder in which the model is saved.

MOC3D ▸ Run...

The available settings of the **Run Moc3d** dialog box (Fig. 3.39) are described below.

- **Moc3d Program** gives the full path and filename of the executable code of MOC3D. PMWIN automatically installs a version of MOC3D in *pmhome*\moc3d\moc3d.exe, where *pmhome* is the folder in which PMWIN is installed. If you want to use another version of Moc3d, click the **open file** button  and select the desired program from a dialog box.
- **The File Table:** PMWIN uses the user-specified data to generate input files of MODFLOW and MOC3D. **Description** gives the name of the packages used in the flow model. The path and name of the input file are shown in **Destination File**. PMWIN generates an input file, only if the **Generate** flag is checked. You may click on a flag to check or uncheck it. Generally, you do not need to worry about these flags, as PMWIN will take care of the settings.
- **Options**:

  Regenerate all input files: You should check this option, if the input files have been deleted or overwritten by other programs.

  Check the model data: Before creating data files for MODFLOW, PMWIN will check the geometry of the model and the consistency of the model data given in table 3.5, if this option is checked. The errors (if any) are saved in the file CHECK.LST located in the same folder as your model data.

  Generate input files only, don't start MOC3D: Check this option, if you do not want to run MOC3D. You can start the simulation at a later time by executing the batch file MOC3D.BAT.

- **OK**: Click **OK** to start the generation of input files for MODFLOW and MOC3D. In addition, PMWIN generates a batch file MOC3D.BAT saved in your model folder. When all necessary files are generated, PMWIN automatically runs MOC3D.BAT in a DOS-window. During a simulation, MOC3D writes a detailed run record to the listing file MOC3D.LST. MOC3D saves the simulation results in various files only if a transport simulation has been successfully completed. See **MOC3D ▸ Output Control** for details about the output terms and the corresponding result files from MOC3D.

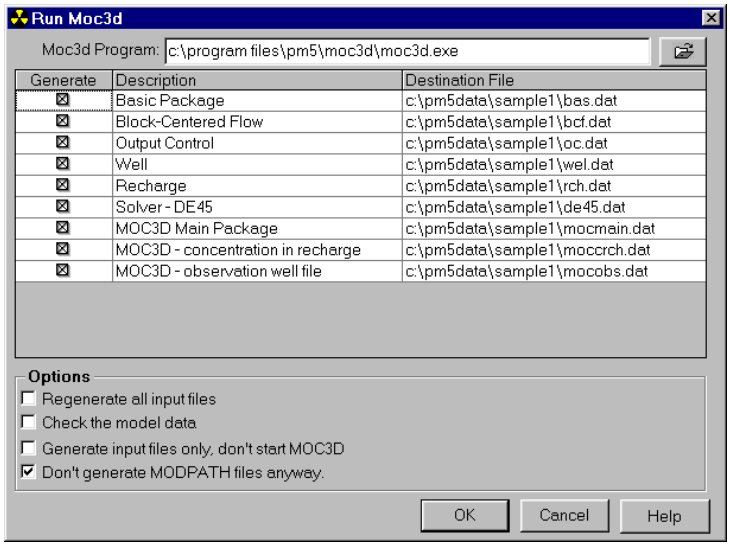


Fig. 3.39 The **Run Moc3d** dialog box

3.6.3 MT3D

MT3D ▸ Initial Concentration

MT3D requires the initial concentration of each active concentration cell, i.e. ICBUND > 0, at the beginning of a transport simulation. The values specified here are shared with MOC3D.

MT3D ▸ Advection...

The available settings of the **Advection Package (MTADV1)** dialog box (Fig. 3.40) are described below. Note that some of the simulation parameters are only required when a particular solution scheme is selected.

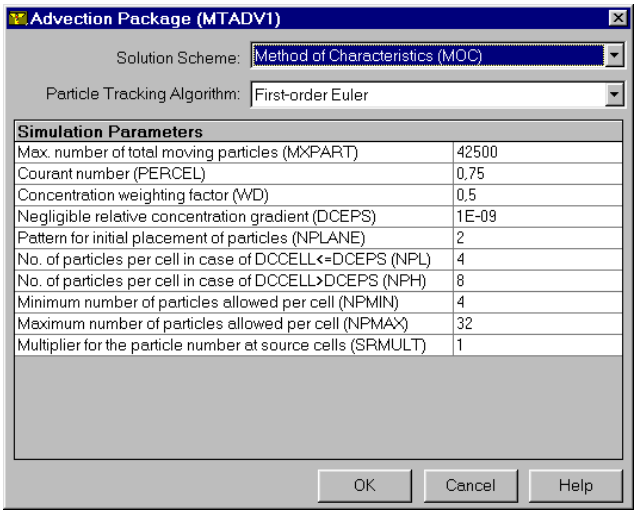


Fig. 3.40 The **Advection Package (MTADV1)** dialog box

- **Solution Scheme**: MT3D provides four solution schemes for the advection term, including the method of characteristics (MOC), modified method of characteristics (MMOC), hybrid method of characteristics (HMOC) and upstream finite difference method.

  The method of characteristics (MOC) scheme (see **MOC3D▸Advection...**) was implemented in the transport models MOC (Konikow and Bredehoeft, 1978) and MOC3D, and has been widely used. One of the most desirable features of the MOC technique is that it is virtually free of numerical dispersion, which creates serious difficulty in many numerical schemes. The major drawback of the MOC scheme is that it can be slow and requires a large amount of computer memory when a large number of particles is required.

  The modified method of characteristics (MMOC) uses one particle for each finite-difference cell and is normally faster than the MOC technique. At each new time level, a particle is placed at the nodal point of each finite-difference cell. The particle is tracked backward to find its position at the old time level. The concentration associated with that position is used to approximate the advection-relevant average concentration at the cell, where the particle is placed. The MMOC technique is free of artificial oscillations if implemented with a lower-order velocity interpolation scheme (such as linear interpolation used in MT3D and MT3DMS). However, with a lower-order velocity interpolation scheme, the MMOC technique introduces some numerical dispersion, especially for sharp front problems.

  The hybrid method of characteristics (HMOC) attempts to combine the strengths of the MOC and MMOC schemes by using an automatic adaptive scheme conceptually similar to the one proposed by Neuman (1984). The fundamental idea behind the scheme is automatic adaptation of the solution process to the nature of the concentration field. When sharp

concentration fronts are present, the advection term is solved by MOC through the use of moving particles dynamically distributed around each front. Away from such fronts, the advection term is solved by MMOC. The criterion for controlling the switch between the MOC and MMOC schemes is given by DCHMOC (see below).

Because of the problems of numerical dispersion and artificial oscillation, the upstream finite difference method is only suitable for solving transport problems not dominated by advection. When the grid Peclet number Pe (Pe = $\Delta x/\alpha_L$; Δx is the grid spacing and α_L is the longitudinal dispersivity) is smaller than two, the upstream finite difference method is reasonably accurate. It is advisable to use the upstream finite difference method anyway for obtaining first approximations in the initial stages of a modeling study.

- **Particle Tracking Algorithm:** MT3D provides three particle tracking options: a **first-order Euler** algorithm, a **fourth-order Runge-Kutta** algorithm, and a combination of these two.

  Using the first-order Euler algorithm, numerical errors tend to be large unless small transport steps are used. The allowed transport step Δt of a particle is determined by MT3D using eq. 3.36.

$$|\Delta t| \leq \gamma_c \cdot R \cdot MIN\left[\frac{\Delta x}{v_x}, \frac{\Delta y}{v_y}, \frac{\Delta z}{v_z}\right] \qquad (3.36)$$

  where Δx, Δy and Δz are the cell widths in the x, y, and z-directions; γ_c is the Courant number. The particle velocities v_x, v_y and v_z at (x, y, z) are obtained by linear interpolation from the specific discharges at the cell faces. The minimum Δt of all particles is used in a transport step.

  The basic idea of the fourth-order Runge-Kutta method is to calculate the particle velocity four times for each tracking step: one at the initial point, twice at two trial midpoint, and once at a trial end point. A weighted velocity based on values evaluated at these four points is used to move the particle to a new position. The fourth-order Runge-Kutta method permits the use of larger tracking steps. However, the computational effort required by the fourth-order Runge-Kutta method is considerably larger than that required by the first-order Euler method. For this reason a mixed option combining both methods is introduced in MT3D. The mixed option is implemented by automatic selection of the fourth-order Runge-Kutta algorithm for particles located in cells which contain or are adjacent to sinks or sources, and automatic selection of the first-order Euler algorithm for particles located elsewhere.
- **MXPART** is the maximum number of particles allowed in a simulation.
- **PERCEL** is the Courant number, or number of cells (or a fraction of a cell) any particle will be allowed to move in any direction in one transport step. Generally, $0.5 \leq \text{PERCEL} \leq 1$.
- **WD** is a concentration weighting factor between 0 and 1. The value of 0.5 is normally a good

choice. This number can be adjusted to achieve better mass balance. Generally, it can be increased toward 1 as advection becomes more dominant.

- **DCEPS** is a criterion for placing particles. A value around 10^{-5} is generally adequate. If DCEPT is greater than the *relative cell concentration gradient* $DCCELL_{j,i,k}$ (eq. 3.37), the higher number of particles NPH is placed in the cell [j, i, k], otherwise the lower number of particles NPL is placed (see NPH and NPL below).

$$DCCELL_{j,i,k} = \frac{CMAX_{j,i,k} - CMIN_{j,i,k}}{CMAX - CMIN} \tag{3.37}$$

where $CMIN_{j,i,k}$ and $CMAX_{j,i,k}$ are the minimim and maximum concentrations in the immediate vicinity of the cell [j, i, k]; CMIN and CMAX are the minimum and maximum concentration in the entire grid, respectively.

- **NPLANE** is a flag indicating whether the random or fixed pattern is selected for initial placement of moving particles.
  - **NPLANE = 0**, the random pattern is selected for initial placement. Particles are distributed randomly in both the horizontal and vertical directions (Fig. 3.41b). This option generally leads to smaller mass balance discrepancy in nonuniform or diverging/converging flow fields.
  - **NPLANE > 0**, the fixed pattern is selected for initial placement. The value of NPLANE serves as the number of vertical "planes" on which initial particles are placed within each cell block (Fig. 3.41a). This fixed pattern may work better than the random pattern only in relatively uniform flow Fields. For two-dimensional simulations in plan view, set NPLANE=1. For cross sectional or three-dimensional simulations, NPLANE=2 is normally adequate. Increase NPLANE if more resolution in the vertical direction is desired.
- **NPL** is the number of initial particles per cell to be placed at cells where the relative cell concentration gradient DCCELL is less than or equal to DCEPS. Generally, NPL can be set to zero since advection is considered insignificant under the condition DCCELL$\leq$DCEPS. Setting NPL equal to NPH causes a uniform number of particles to be placed in every cell over the entire grid (i.e., the uniform approach).
- **NPH** is the number of initial particles per cell to be placed at cells where the relative cell concentration gradient DCCELL is greater than DCEPS. The selection of NPH depends on the nature of the flow field and also the computer memory limitation. Generally, use a smaller number in relatively uniform flow fields and a larger number in relatively nonuniform flow fields. However, values exceeding 16 in two-dimensional simulations or 32 in three-dimensional simulations are rarely necessary. If the random pattern is chosen, NPH

particles are randomly distributed within the cell block. If the fixed pattern is chosen, NPH is divided by NPLANE to yield the number of particles to be placed per plane, which is rounded to one of the values shown in Fig. 3.42.

- **NPMIN** is the minimum number of particles allowed per cell. If the number of particles in a cell at the end of a transport step is fewer than NPMIN, new particles are inserted into that cell to maintain a sufficient number of particles. NPMIN can be set to 0 in relatively uniform flow fields, and a number greater than zero in diverging/converging flow fields. Generally, a value between zero and four is adequate.
- **NPMAX** is the maximum number of particles allowed per cell. If the number of particles in a cell exceeds NPMAX, particles are removed from that cell until NPMAX is met. Generally, NPMAX can be set to approximately twice NPH.
- **SRMULT** is a multiplier for the particle number at source cells (SRMULT≥1). In most cases, SRMULT=1 is sufficient. However, better results may be obtained by increasing SRMULT.
- **NLSINK** is a flag indicating whether the random or fixed pattern is selected for initial placement of particles to approximate sink cells in the MMOC scheme. The convention is the same as that for NPLANE. It is generally adequate to set NLSINK equivalent to NPLANE.
- **NPSINK** is the number of particles used to approximate sink cells in the MMOC scheme. The convention is the same as that for NPH. It is generally adequate to set NPSINK equivalent to NPLANE.
- **DCHMOC** is the critical relative concentration gradient for controlling the selective use of either MOC or MMOC in the HMOC solution scheme. The MOC solution is selected at cells where the relative cell concentration gradient DCCELL is greater than DCHMOC. The MMOC solution is selected at cells where the relative cell concentration gradient DCCELL is lessr than or equal to DCHMOC.

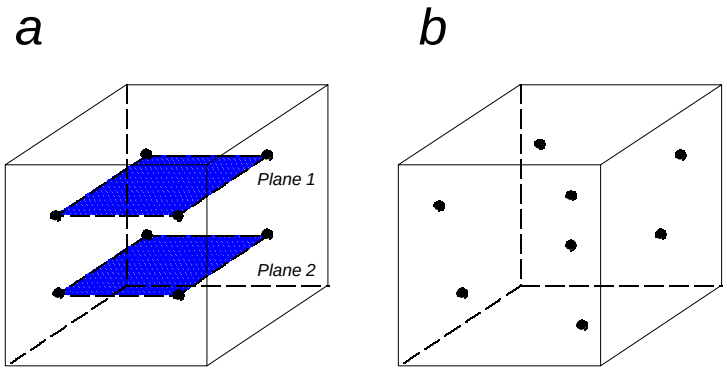


Fig. 3.41 Initial placement of moving particles (adopted from Zheng, 1990).
(a) Fixed pattern, 8 particles are placed on two planes within the cell block
(b) Random pattern, 8 particles are placed randomly within the cell block

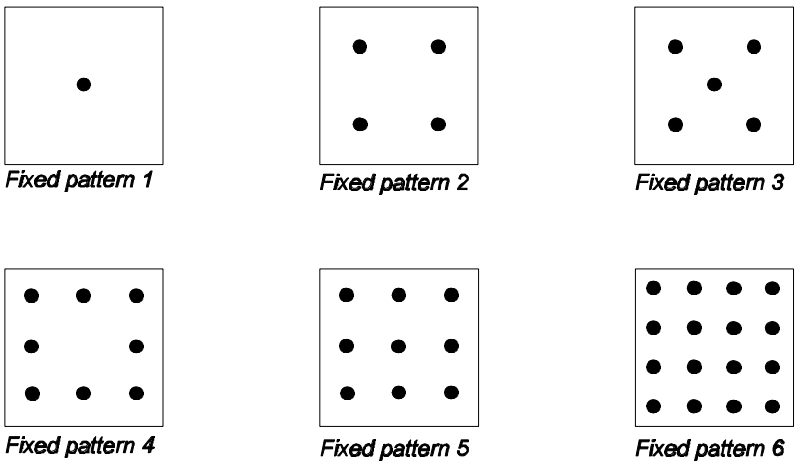


Fig. 3.42 Distribution of initial particles using the fixed pattern (adopted from Zheng, 1990) If the fixed pattern is chosen, the number of particles placed per cell (NPL and NPH) is divided by the number of vertical planes NPLANE, to yield the number of particles to be placed on each vertical plane, which is then rounded to one of the numbers of particles shown here.

MT3D ▸ Dispersion...

The following values must be specified for each layer in the **Dispersion Package (MT3D/MT3DMS)** dialog box (Fig. 3.43). The longitudinal dispersivity for each finite-difference cell is specified in the **Data Editor**.

- **TRPT** is the ratio of the horizontal transverse dispersivity to the longitudinal dispersivity.
- **TRPV** is the ratio of the vertical transverse dispersivity to the longitudinal dispersivity.
- **DMCOEF** is the effective molecular diffusion coefficient D* [L^2T^{-1}] (see eq. 3.34).

Refer to **MOC3D ▸ Dispersion & Chemical Reaction...** for more about the molecular diffusion coefficient and dispersivity.

In MT3D, the concentration change due to dispersion alone is solved with a fully explicit central finite-difference scheme. There is a certain stability criterion associated with this scheme. To retain stability, the transport step size cannot exceed an upper limit defined by eq. 3.38.

$$\Delta t \leq \frac{0.5 \cdot R}{\frac{D_{xx}}{\Delta x^2} + \frac{D_{yy}}{\Delta y^2} + \frac{D_{zz}}{\Delta z^2}} \qquad (3.38)$$

where Δx, Δy and Δz are the widths of the cell in the x, y and z-directions; R is the retardation factor. The components of the hydrodynamic dispersion coefficient D_{xx}, D_{yy} and D_{zz} are calculated by eq. 3.39.

$$
\begin{aligned}
D_{xx} &= \alpha_L \cdot \frac{v_x^2}{|v|} + \alpha_{TH} \cdot \frac{v_y^2}{|v|} + \alpha_{TV} \cdot \frac{v_z^2}{|v|} + D^* \\
D_{yy} &= \alpha_L \cdot \frac{v_y^2}{|v|} + \alpha_{TH} \cdot \frac{v_x^2}{|v|} + \alpha_{TV} \cdot \frac{v_z^2}{|v|} + D^* \\
D_{zz} &= \alpha_L \cdot \frac{v_z^2}{|v|} + \alpha_{TV} \cdot \frac{v_x^2}{|v|} + \alpha_{TV} \cdot \frac{v_y^2}{|v|} + D^*
\end{aligned}
\qquad (3.39)
$$

where α_L [L] is the longitudinal dispersivity; α_{TH} [L] is the horizontal transverse dispersivity; α_{TV} [L] is the vertical transverse dispersivity; v_x, v_y, v_z [LT^{-1}] are components of the flow velocity vector along the x, y, and z axes; and

$$|v| = (v_x^2 + v_y^2 + v_z^2)^{1/2} \qquad (3.40)$$

Eq. 3.38 is calculated for each active cell and the minimum Δt is taken as the maximum allowed step size for solving the dispersion term. This criterion is compared with other transport step size constraints to determine the minimum step size for the simulation. Generally, a higher flow velocity, for example the velocity in the immediate vicinity of a pumping well, will cause larger values of D_{xx}, D_{yy} and D_{zz}, which, in turn, result in a smaller Δt in eq. 3.38. When Δt is too small, the required CPU-time will become enormous. To overcome this problem, an implicit formulation is implemented in MT3DMS. See section 3.6.4 for details.

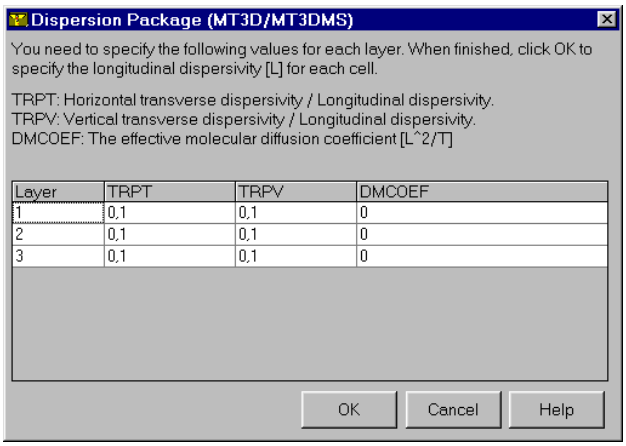


Fig. 3.43 The **Dispersion Package (MT3D/MT3DMS)** dialog box

MT3D ▸ Chemical Reaction ▸ Layer by Layer

Chemical reactions supported by MT3D include equilibrium-controlled sorption and first-order irreversible rate reactions, such as radioactive decay or biodegradation. It is generally assumed that equilibrium conditions exist between the aqueous-phase and solid-phase concentrations and that the sorption reaction is fast enough relative to groundwater velocity so that it can be treated as instantaneous. Consider to use MT3DMS, if nonequilibrium (rate-limited) sorption needs to be simulated.

Use this menu item to open the **Chemical Reaction Package (MTRCT1)** dialog box (Fig. 3.44) to specify the required parameters on a layer-by-layer basis. The parameters are described below.

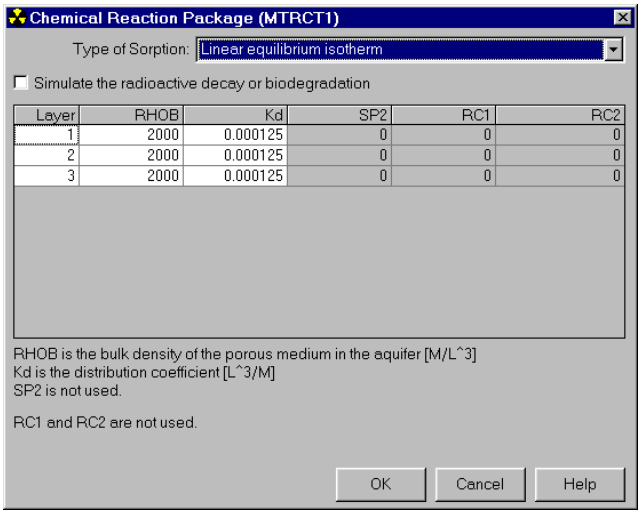


Fig. 3.44 The **Chemical Reaction Package (MTRCT1)** dialog box

- **Type of sorption**: Sorption is implemented in MT3D through use of the retardation factor R. MT3D provides three types of sorptions: the linear equilibrium isotherm, Freundlich nonlinear equilibrium isotherm and Langmuir nonlinear equilibrium isotherm.

  The **linear sorption** isotherm assumes that the sorbed concentration $\bar{C}_{j,i,k}$ is directly proportional to the dissolved concentration $C_{j,i,k}$ (eq. 3.41) and the retardation factor is independent of the concentration field. The retardation factor is calculated only once for each cell at the beginning of the simulation by eq. 3.42.

$$\bar{C}_{i,j,k} = K_d \cdot C_{j,i,k} \tag{3.41}$$

$$R_{j,i,k} = 1 + \frac{\rho_b}{n_{j,i,k}} \cdot K_d \tag{3.42}$$

where $n_{j,i,k}$ [-] is the porosity of the porous medium in the cell [j, i, k]; K_d [L^3M^{-1}] is the distribution coefficient that depends on the solute species, nature of the porous medium, and other conditions of the system; and ρ_b [ML^{-3}] is the bulk density of the porous medium. The bulk density is the ratio of the mass of dried soil to total volume of the soil.

The **Freundlich** isotherm is a non-linear isotherm, which can be expressed in eq. 3.43. The retardation factor at the beginning of each transport step is calculated by eq. 3.44.

$$\bar{C}_{j,i,k} = K_f \cdot C_{j,i,k}^{a} \tag{3.43}$$

$$R_{j,i,k} = 1 + \frac{\rho_b}{n_{j,i,k}} \cdot a \cdot C_{j,i,k}^{a-1} \cdot K_f \tag{3.44}$$

where $C_{j,i,k}$ is the solute concentration in the cell in the cell [j, i, k] at the beginning of each transport step; a [-] is the Freundlich exponent; and K_f [L^3M^{-1}] is the Freundlich constant.

The **Langmuir** non-linear sorption isotherm is described by eq. 3.45. The retardation factor at the beginning of each transport step is calculated by 3.46.

$$\bar{C}_{j,i,k} = \frac{K_L \cdot \bar{S} \cdot C_{j,i,k}}{1 + K_L \cdot C_{j,i,k}} \tag{3.45}$$

$$R_{j,i,k} = 1 + \frac{\rho_b}{n_{j,i,k}} \cdot \frac{K_L \cdot \bar{S}}{(1 + K_L \cdot C_{j,i,k})^2} \tag{3.46}$$

where K_L [L^3M^{-1}] is the Langmuir constant and $\bar{S}$[MM^{-1}] is the maximum amount of the solute that can be adsorbed by the soil matrix.

For more information on the mathematical description of adsorption and transport of reactive solutes in soil, the user can refer to Travis (1978) or Bear and Verruijt (1987).

- **Simulate the radioactive decay or biodegradation**: Check this box to simulate the effect of the first-order irreversible rate reactions. The concentration change due to the chemical reaction from one transport step to another transport step at cell [j, i, k] can be expressed as

$$\Delta C_{RCT\ i,j,k} = -\frac{\Delta t}{R_{i,j,k}} \cdot \left(\lambda_1 \cdot C_{i,j,k} + \lambda_2 \cdot \frac{\rho_b}{n_{i,j,k}} \cdot \bar{C}_{i,j,k} \right) \tag{3.47}$$

where λ_1 [T^{-1}] is the first-order rate constant for the dissolved phase; λ_2 [T^{-1}] is the first-order rate constant for the sorbed phase; Δt is the transport time-step; and $\bar{C}_{j,i,k}$ is the mass of the solute species adsorbed on the solids per unit bulk dry mass of the porous medium at the

beginning of each transport step. $\bar{C}_{j,i,k}$ is in equilibrium with solute concentration $C_{j,i,k}$ in the cell [j, i, k].

The rate constant λ is usually given in terms of the half-life $t_{1/2}$ (see eq. 3.32). Generally, if the reaction is radioactive decay, λ_2 should be set equal to λ_1. However, for certain types of biodegradation, λ_2 may be different from λ_1.

MT3D ▸ Chemical Reaction ▸ Cell by Cell (only MT3D96)

Chemical Reactions Package 2 supported by the MT3D96 transport model includes all functions of the Chemical Reactions Package of MT3D (version 1.xx). Using the **Data Editor**, chemical reaction coefficients may be entered on a three-dimensional cell-by-cell basis. This option provides the ability to have different reaction coefficients for different areas in a single model layer. See **MT3D ▸ Chemical Reaction ▸ Layer by Layer** for details about the parameters.

MT3D ▸ Sink/Source Concentration

This menu is used for specifying the concentration associated with the fluid of point or areally-distributed sources or sinks. The concentration of a particular source or sink is specified by the **Data Editor**. Point sources include wells, general-head boundary cells, fixed-head cells, rivers and streams. Recharge is the only areally-distributed source whereas evapotranspiration is the only sink whose concentration can be specified. Note that MT3D does not allow the concurrent use of the rivers and the streams. This does not cause problems in any case, because the Streamflow-Routing package has all functions of the River package.

The concentration of a sink cannot be greater than that of the aquifer at the sink cell. If the sink concentration is specified greater than that of the aquifer, it is automatically set equal to the concentration of the aquifer.

Menu items of this menu are dimmed if the corresponding hydraulic features given in the **Models▸Modflow** menu are not used (checked). You may or may not specify the concentration for the sources or sinks when they are used in the flow simulation. The specified concentration will be used in the transport simulation if a corresponding menu item is checked. If a checked item is no longer necessary for a transport simulation, simply select the item again and deactivate it. If the concentration of a source or sink is not specified, the default value for the concentration is zero.

Using **Time-Variant Specified-Concentration**, you may define constant-concentration cells anywhere in the model grid and different concentration values can be specified for different stress periods. A time-variant specified-concentration cell is defined by specifying the following data in

the **Data Editor**. Note that **Time-Variant Specified-Concentration** may not be supported by some earlier version of MT3D.

- **Flag [-]**. A non-zero value indicates that a cell is specified as a constant concentration cell. In a multiple stress period simulation, a constant-concentration cell, once defined, will remain a constant-concentration cell in the duration of the simulation, but its concentration value can be specified to vary in different stress period. To change the concentration value in a particular stress period, simply set a non-zero value to **Flag** and assign the desired concentration value to **Specified Concentration**.
- **Specified Concentration** [ML^{-3}]. This value is the concentration in the cell from the beginning of a stress period.

MT3D ▸ Output Control...

Use the **Output Control (MT3D, MT3DMS)** dialog box (Fig. 3.45) to set the output options from MT3D. The options in this dialog box are grouped under three tabs described below.

- **Output Terms**: The MT3D transport model always generates a listing file OUTPUT.MT3, which documents the details of each simulation step. Optionally, you can save other output terms by checking the corresponding output terms in this tab. All output terms denoted by (ASCII) are also saved in the listing file. The calculated concentration values will be saved in the unformatted binary file MT3D.UCN. In addition, MT3D96 can save the mass contained in each cell in the unformatted binary file MT3D.CBM. All output files are located in the same folder as your model. You can use the **Result Extractor** to read the unformatted binary files.
- **Output Times:** The value of the output frequency, NPRS, indicates whether the output is produced in terms of total elapsed simulation time or the transport step number. If NPRS=0, simulation results will only be saved at the end of simulaton. If NPRS<0, simulation results will be saved whenever the number of transport steps is an even multiple of NPRS. If NPRS>0, simulation results will be saved at times as specified in the table as shown in Fig. 3.46. There are two ways for specifying the output times. You may click the table header **Output Time** and then enter a minimum time, a maximum time and a time interval between each output into an **Output Time** dialog box. PMWIN will use these entries to calculate NPRS and the output times. The other way is to specify a positive NPRS and press the **Tab** Key, then enter the output times into the table. Note that the output times are measured from the beginning of the simulation.

- **Misc.**:
  - **CINACT** is the predefined concentration value for an inactive concentration cell (ICBUND=0).
  - **THKMIN** is the minimum saturated thickness in a cell, expressed as the decimal fraction of the model layer thickness, below which the cell is considered inactive. THKMIN will only be used by MT3D96 or later.
  - **NPRMAS** indicates how frequently the mass budget information should be saved in the mass balance summary file MT3D.MAS.

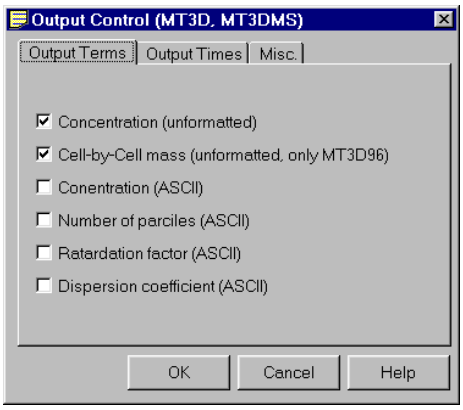


Fig. 3.45 The **Output Control (MT3D, MT3DMS)** dialog box

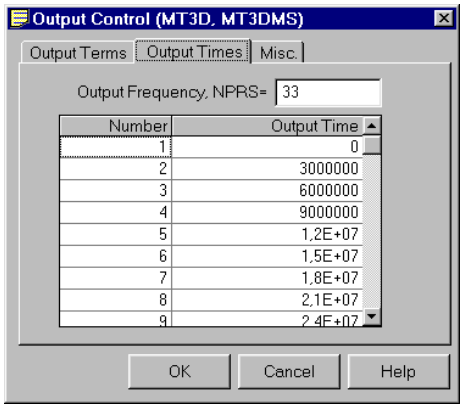


Fig. 3.46 Specifying the **output times** for MT3D

MT3D ▸ Run...

The available settings of the **Run MT3D/MT3D96** dialog box (Fig. 3.47) are described below.

- **MT3D Program** contains the full path and filename of the MT3D code, which will be called

by PMWIN. The default code is the version DoD_1.5 developed by Zheng (1996). If you want to use a compiled version located in another position, click the **open file** button and select the desired code from a dialog box.

- **The File Table:** PMWIN uses the user-specified data to generate input files of MT3D. **Description** gives the name of the packages used in the flow model. The path and name of the input file are shown in **Destination File**. PMWIN generates an input file, only if the corresponding **Generate** flag is checked. You may click on a flag to check or uncheck it. Normally, you do not need to worry about these flags, as PMWIN will take care of the settings.
- **Options**:
  - **Regenerate all input files for MT3D:** You should check this option, if the input files have been deleted or overwritten by other programs.
  - **Regenerate input files only, don't start MT3D:** Check this option, if you do not want to run MT3D. You can start the simulation at a later time by executing the batch file MT3D.BAT.
- **OK**: Click **OK** to start the generation of MT3D input files. In addition, PMWIN generates a batch file MT3D.BAT saved in your model directory. When all necessary files are generated, PMWIN automatically runs MT3D.BAT in a DOS-window. During a flow simulation, MT3D saves results to various output files and writes a detailed run record to the listing file OUTPUT.MT3 saved in your model folder. See **MT3D ▸ Output Control...** for details about the output terms.

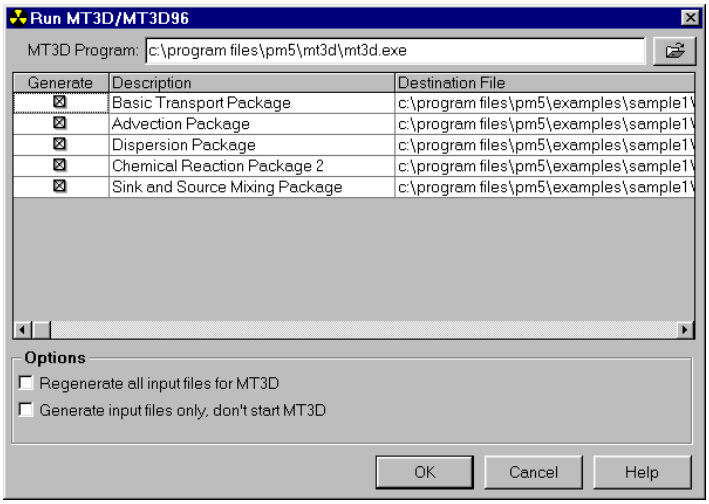


Fig. 3.47 The **Run MT3D/MT3D96** dialog box

3.6.4 MT3DMS

As MT3DMS retains the same modular structure of the MT3D code, the interface implemented in PMWIN is very similar to the MT3D interface. One of the major differences is that you are asked to specify initial concentration, source concentration and parameters for chemical reactions for *each active species* in the **Data Editor**. Before switching to the **Data Editor**, PMWIN will display a dialog box, which allows you to manage the data of each species. For example, if you select **MT3DMS ▸ Initial Concentration...**, the **Initial Concentration (MT3DMS)** dialog box (Fig. 3.48) will appear. You have the following options.

1. Edit the initial concentration data for a species by selecting a row from the table and clicking the **Edit** button. After specifying and saving the data, the **Active** and **Data** flags will be checked.
2. You may click on an **Active** flag to activate or deactivate a species.
3. The **Data** flag offers three status configuration possibilities:
   ☒ - data has been specified and will be used for simulation.
   ☐ - data has been specified, but will not be used; the default value of zero will be used.
   ☐ - data is not available (the flag is dimmed and deactivated).
   Once the data is specified, you may click on a **Data** flag to check or uncheck it.

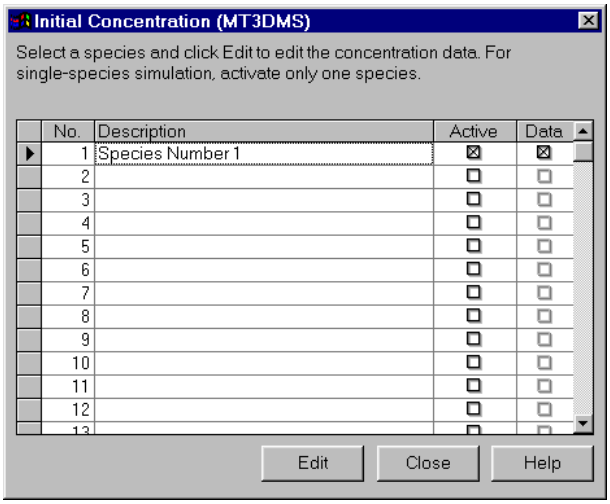


Fig. 3.48 The **Initial Concentration (MT3DMS)** dialog box

MT3DMS ▸ Initial Concentraion...

At the beginning of a transport simulation, MT3DMS requires the initial concentration of each active species at each active concentration cell, i.e. ICBUND > 0.

MT3DMS ▸ Advection...

The available settings of the **Advection Package (MT3DMS)** dialog box (Fig. 3.49) are described below. Note that the simulation parameters, except the Courant number, in the table of this dialog box are only required when the method of characteristics (or its variants, see **MT3D▸Advection...** for details) is selected.

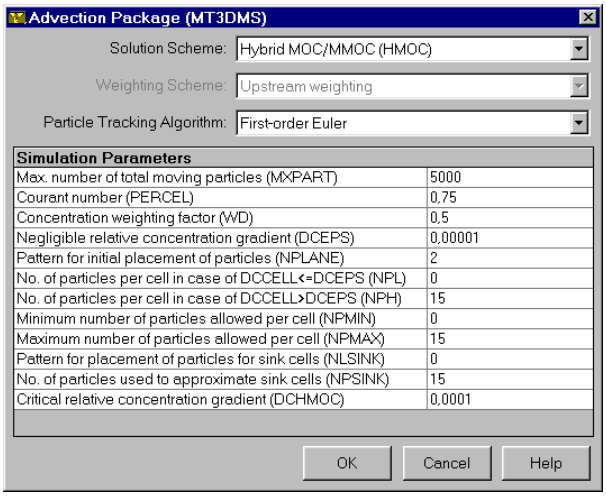


Fig. 3.49 The **Advection Package (MT3DMS)** dialog box

- **Solution Scheme**: MT3DMS provides five solution schemes for the advection term, including the method of characteristics (MOC), modified method of characteristics (MMOC), hybrid method of characteristics (HMOC), upstream finite difference method and third-order TVD method (ULTIMATE). The first three methods are the same as in MT3D.

  The **finite-difference method** can be explicit as in MT3D or fully implicit without any stability constraint to limit transport step sizes. The finite-difference solution is implicit when the Generalized Conjugate Gradient solver (GCG) package is activated (see **MT3DMS▸Solver▸GCG...**).

  The **third-order TVD method** is based on the ULTIMATE algorithm (Leonard, 1988; Leonard and Niknafs, 1990, 1991), which is in turn derived from the earlier QUICKEST algorithm (Leonard, 1979). With the ULTIMATE scheme, the solution is mass conservative, without excessive numerical dispersion and artificial oscillation.

- **Weighting Scheme** is needed only when the implicit finite-difference method is used, i.e., the solution scheme is finite-difference and the iterative GCG solver is used. In the finite-difference method, when computing the mass flux into a model cell by advection, the concentration values at the cell interfaces between two neighboring cells are used. For the **upstream weighting** scheme, the interface concentration in a particular direction is equal to the concentration at the upstream node along the same direction. For the **central-in-space weighting** scheme, the interface concentration is obtained by linear interpolation of the concentrations at the two neighboring cells.

  As denoted in Zheng and Wang (1998), the central-in-space scheme does not lead to intolerable numerical dispersion when the grid spacing is regular. However, if transport is dominated by advection, the upstream weighting is preferred, as the central-in-space weighting scheme can lead to excessive artificial oscillation.
- **Particle Tracking Algorithm** is used in combination with the method of characteristics. The particle tracking options are the same as provided in MT3D.

MT3DMS ▸ Dispersion...

MT3DMS and MT3D share the same dispersion parameters. See **MT3D▸Dispersion...** for details about the parameters.

In MT3DMS, the concentration change due to dispersion alone can be solved with a fully explicit central finite-difference scheme or an implicit (upstream or central) finite-difference scheme with the Generlized Conjugate Gradient solver. The implicit method does not have any stability constraint.

MT3DMS ▸ Chemical Reaction...

The required parameters are specified in the **Chemical Reaction (MT3DMS)** dialog box (Fig. 3.50) of the **Data Editor.** Chemical reactions supported by MT3DMS include equilibrium-controlled sorption, non-equilibrium sorption and first-order irreversible rate reactions, such as radioactive decay or biodegradation. The equilibrium-controlled sorption and first-order irreversible rate reactions are essentially the same as in MT3D (see **MT3D▸Chemical Reaction▸Layer by Layer...)**. It should be noted that the basic chemical reaction supported by the present version of MT3DMS is intended for single-species systems. More sophisticated reaction models such as RT3D (Clement, 1997) or TBC (Schäfer et al., 1997) should be used for multi-species reactions.

Three new options, the first-order kinetic sorption and the dual-domain mass transfer with

or without sorption, are described below. Using these options, you have the choice of specifying the initial concentration for the sorbed or immobile phase for each species. To do this, simple check **Use the initial concentration for the nonequibrilium sorbed or immobile liquid phase** and specify the concentration value to **Initial concentration for the sorbed phase** or **Initial concentration for the immobile liquid phase** in the **Chemical Reaction (MT3DMS)** dialog box.

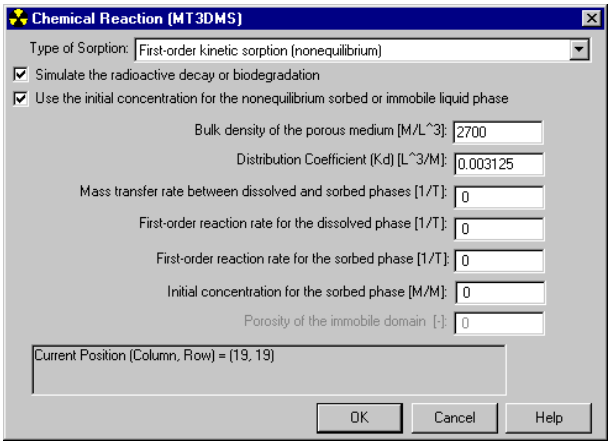


Fig. 3.50 The **Chemical Reaction (MT3DMS)** dialog box

- **First-order kinetic sorption:** When the local equilibrium assumption is not valid, it is assumed in MT3DMS that sorption can be represented by a **first-order reversible kinetic sorption** described by

$$\rho_b \cdot \frac{\partial \bar{C}}{\partial t} = \beta \left(C - \frac{\bar{C}}{K_d} \right) \tag{3.48}$$

where β [T^{-1}] is the first-order mass transfer rate between the dissolved and sorbed phases, ρ_b [ML^{-3}] is the bulk density of the porous medium, $\bar{C}$ is the sorbed concentration and K_d [L^3M^{-1}] is the distribution coefficient as defined previously in eq. 3.41.

Eq. 3.48 can be rearranged in

$$C - \frac{\bar{C}}{K_d} = \frac{\rho_b}{\beta} \cdot \frac{\partial \bar{C}}{\partial t} \tag{3.49}$$

If sufficient time is available for the system to reach equilibrium (for example, the flow velocity of groundwater is very slow), then there is no further change in $\bar{C}$ and $\partial \bar{C} / \partial t = 0$, so that eq. 3.49 is reduced to linear sorption (eq. 3.41). If the first-order mass transfer rate

is infinitely large, the right-hand side of eq. 3.49 is equal to zero, which also leads to linear sorption. For very small values of β, the left-hand-side of eq. 3.48 becomes negligible, i.e., there is no change in the sorbed concentration and sorption is negligible.

- **First-order kinetic dual-domain mass transfer:** Dual-domain means that two kinds of continuum, e.g. a fractured medium and the porous medium, exist simultaneously in the same spatial region, i.e., the same model cell. In fractured aquifers, the water moves faster along fractures than it does in a rock formation and the solute transport is often controlled by advection along the fractures and dominated by dispersion in the porous block along the fractures.

  MT3DMS uses the dual-domain concept to approach extremely heterogeneous porous media or media composed of fractures and pores. In this approach, the effective porosity specified in **Parameters▸Effective Porosity** is used as the primary porosity for the pore spaces filled with mobile water (i.e., fractures) and the secondary porosity for the pore spaces filled with immobile water (i.e., rock formation) is defined in the **Chemical Reaction (MT3DMS)** dialog box (Fig. 3.50). The sum of the primary and the secondary porosities is the total porosity of the medium. The exchange of solutes between the mobile and immobile domains can be defined through eq. 3.50.

$$n_{im} \cdot \frac{\partial C_{im}}{\partial t} = \zeta \cdot (C_m - C_{im}) \qquad (3.50)$$

where n_{im} [-] is the secondary porosity (i.e., the portion of total porosity filled with immobile water); C_m [ML^{-3}] is the concentration in the mobile domain; C_{im} [ML^{-3}] is the concentration in the immobile domain; and ζ [T^{-1}] is the first-order mass transfer rate between the mobile and immobile domains.

As the mass transfer rate ζ increases, the dual-domain model functions more and more like the single-domain model with a porosity approaching the total porosity of the porous medium. For very small values of ζ, the right-hand-side of eq. 3.50 approaches zero, i.e., there is no change of the concentration in the immobile domain and the model functions like a single-porosity model with the primary effective porosity.

One of the advantages of this approach is that the fracture structure does not need to be known. However, a problem may arise when one tries to estimate the mass transfer rate ζ by measuring the concentrations C_m and C_{im}. When we measure the concentration at a certain point, we only obtain one value and cannot distinguish between mobile and immobile concentration. It is therefore more likely that ζ must be estimated through a model calibration using C_m values only.

MT3DMS ▸ Sink/Source Concentration

The use of this menu is the same as **MT3D▸Sink/Source Concentration**, except the use of **Time-Variant Specified-Concentration.** A time-varying specified-concentration cell is defined by setting the following data in the **Data Editor**.

- **Flag [-]**. A non-zero value indicates that a cell is specified as a constant concentration cell.
- **Specified Concentration** [ML^{-3}]. This value is the concentration in the cell from the beginning of a stress period.

In a *multiple stress period* simulation, a constant-concentration cell, once defined, will remain a constant-concentration cell during the simulation, but its concentration value can be specified to vary in different stress period. To change the concentration value in a particular stress period, simply set a non-zero value to **Flag** and assign the desired concentration value to **Specified Concentration**.

*In a multispecies simulation, the **Flag** is applied to all species.* If the constant-concentration condition does not apply to a particular species, assign a *negative* concentration value for the species. The negative value is used by MT3DMS to skip assigning the constant-concentration for the designated species.

MT3DMS ▸ Mass-Loading Rate

Instead of specifying a source concentration associated with a fluid source, the mass-loading rate [MT^{-1}] into the groundwater system can directly be specified by using this menu item.

MT3DMS ▸ Solver ▸ GCG...

MT3DMS includes a general-purpose iterative solver based on the generalized conjugate gradient method for solving the system of the transport equations. The solver is implemented in the **Generalized Conjugate Gradient** package. A detailed description of the method can be found in Zheng and Wang (1998).

If this solver is activated (i.e., the menu item is checked; you can uncheck the item by selecting it again), dispersion, sink/source, and reaction terms are solved implicitly without any stability constraints. The required settings and parameters for this package are specified in the **Generalized Conjugate Gradient (GCG)** dialog box (Fig. 3.51).

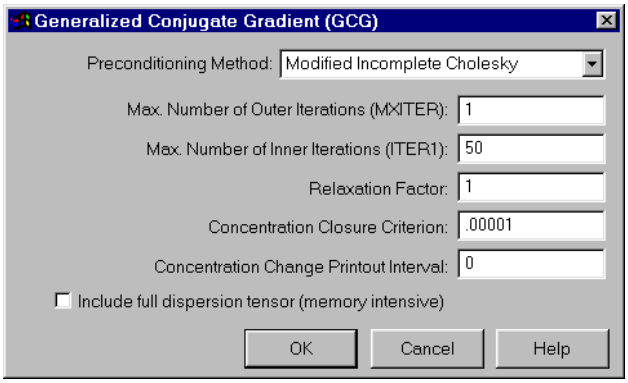


Fig. 3.51 The **Generalized Conjugate Gradient (GCG)** dialog box

- **Preconditioning Method**: The GCG package has three preconditioning options: Jacobi, Symmetric Successive Overrelaxation (SSOR), and the Modified Incomplete Cholesky (MIC). The MIC preconditioner usually takes fewer iterations than the other methods, but it requires significantly more memory.
- **Max. Number of Outer Iterations (MXITER)** and **Max. Number of Inner Iterations (ITER1)**: The GCG solver has two iteration loops, an inner loop and an outer loop. Like the PCG2 solver of MODFLOW (see **MODFLOW▸Solvers▸PCG2**), within the inner loop all coefficients in the (transport-) matrix $\underline{A}$ and the right-hand-side vector ($\underline{b}$) remain unchanged during inner iterations. The inner loop continues until ITER1 - iterations are executed or the convergence criterion is met. If some of the coefficients in $\underline{A}$ are dependent on the concentration being solved, as in the case of nonlinear sorption, they must be updated in outer iterations. So, **MXITER** should be set to an integer greater than one only when a nonlinear sorption isotherm is included in the simulation. For **ITER1**, a value between 30 and 50 should be adequate for most problems.
- **Relaxation Factor** is only used for the SSOR option, a value of 1.0 is generally adequate.
- **Concentration Closure Criterion** is the convergence criterion, a value between 10^{-4} and 10^{-6} is generally adequate. Before solving the system of transport equations, it is normalized by dividing the concentration terms by the maximum concentration of all cells. When the change of the normalized concentration at all cells during a inner iteration is less than or equal to this value, iteration stops. When it takes only one inner iteration to converge, the solution is considered to have converged and the simulation proceeds to the next transport step.
- **Concentration Change Printout Interval:** The maximum concentration changes is printed out whenever the iteration number is an even multiple of this printout interval. Set it to zero for printing only at the end of each stress period.
- **Include full dispersion tensor (memory intensive)**: This is a flag for treatment of dispersion tensor cross terms. If this option is not used, all dispersion cross terms will be

lumped to the right-hand-side of the system of transport equations. Omitting the cross terms represents a method of approximation which is highly efficient.

MT3DMS ▸ Output Control...

MT3DMS and MT3D have the same output structure. See **MT3D▸Output Control...** for the use of the **Output Control (MT3D, MT3DMS)** dialog box (Fig. 3.44)

MT3DMS ▸ Run...

The available settings of the **Run MT3DMS** dialog box (Fig. 3.52) are described below.

- **MT3DMS Program** contains the full path and filename of the MT3DMS code, which will be called by PMWIN. The default code is the version *DoD_3.00.A* developed by Zheng and Wang (1998). If you want to use a compiled version located in an other position, click the **open file** button  and select the desired code from a dialog box.
- **The File Table:** PMWIN uses the user-specified data to generate input files of MT3D. **Description** gives the name of the packages used in the flow model. The path and name of the input files are shown in **Destination File**. PMWIN generates an input file, only if the corresponding **Generate** flag is checked. You may click on a flag to check or uncheck it. Normally, you do not need to worry about these flags, as PMWIN will take care of the settings.
- **Options**:
  Regenerate all input files for MT3DMS: You should check this option, if the input files have been deleted or overwritten by other programs.
  Generate input files only, don't start MT3DMS: Check this option, if you do not want to run MT3DMS. You can start the simulation at a later time by executing the batch file MT3DMS.BAT.
- **OK**: Click **OK** to start the generation of MT3DMS input files. In addition, PMWIN generates a batch file MT3DMS.BAT saved in your model directory. When all necessary files are generated, PMWIN automatically runs MT3DMS.BAT in a DOS-window. During a flow simulation, MT3DMS saves results to various output files and writes a detailed run record to the listing file OUTPUT.MTM saved in your model folder.

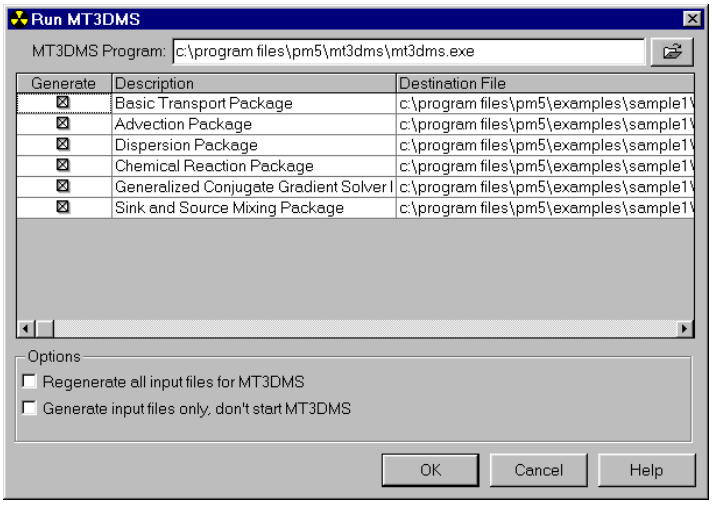


Fig. 3.52 The **Run MT3DMS** dialog box

3.6.5 PEST (Inverse Modeling)

This menu provides an interface between PMWIN, the flow model MODFLOW and the inverse model PEST. Depending on the layer type (see **Grid▸Layer Type...**), the parameters and/or excitations listed in Table 3.7 can be adjusted until model-generated numbers fit the observation values as closely as possible. That is, PEST searches a parameter set for which the sum of squared deviations between model-calculated and measurement values at the observation boreholes is reduced to a minimum. The coordinates of the observation boreholes and measurement values are given in **Parameters ▸ Boreholes and Observations**. A simultaneous fit of highly correlated parameters, for example transmissivities and recharge, is of little value in steady-state problems due to the non-uniqueness of such a fit.

▸ **To define an estimated parameter**

1. From the **Parameters** or **Models▸Modflow** menu, select a parameter or a package, for example *Horizontal Hydraulic Conductivity* or *Well*.
2. Assign a unique parameter number to cells within an area where the parameter value will be estimated. If you intend to calibrate the pumping rate of wells or the conductance of head-dependent cells (e.g., drain, general head-boundary, river or stream cells) for example, you must also assign a non-zero pumping rate or conductance to those cells. Pumping rate or conductance values will not be adjusted, if the user-specifed values are equal to zero.
3. Use the **List of Calibration Parameters (PEST)** dialog box to activate the estimated parameter and to specify the necessary values.

Note that for layers of type **0:confined** and **2:confined/unconfined (transmissivity=const.)**, MODFLOW reads transmissvity (instead of hydraulic conductivity) from the model data file. Consequently, you are actually calibrating the transmissivity value as an estimated parameter defined within horizontal hydraulic conductivity. For multi-layer models, MODFLOW requires vertical leakance (instead of vertical hydraulic conductivity, which is used by PMWIN to calculate the vertical leakance for MODFLOW). Due to this fact, automatic fit of vertical hydraulic conductivity cannot be done without modifying the inverse model or MODFLOW. So, if you assign an estimated parameter within vertical hydraulic conductivity, you should keep in mind that you are actually calibrating the vertical leakance between two layers (the layer with the estimated parameter and the underlying layer).

Table 3.7 Adjustable parameters through an automatic calibration within PMWIN

Layer / types / Parameter or excitations	0	1	2	3
Transmissivity	yes	no	yes	no
Horizontal hydraulic conductivity	no	yes	no	yes
Vertical leakance	yes	yes	yes	yes
Specific yield (only if the simulation is transient)	no	yes	yes	yes
Confined storage coefficient (only if the simulation is transient)	yes	no	yes	yes
Pumping or injection rates of wells	yes	yes	yes	yes
Conductance of drain, general-head boundary, river or stream cells	yes	yes	yes	yes
Recharge flux	yes	yes	yes	yes
Maximum evapotranspiration rate	yes	yes	yes	yes
Inelastic storage factor (only if the simulation is transient and the Interbed Storage package is used)	yes	yes	yes	yes

PEST (Inverse Modeling) ▸ Parameter List...

The required inputs and options for the PMWIN/MODFLOW/PEST interface are specified in the **List of Calibration Parameters (PEST)** dialog box (Fig. 3.53). The avaliable settings are grouped under five tabs described below. Using the **Save...** or **Load...** button, you can save or load the settings.

- **Parameters:** The table gives an overview of the initial values and properties of each estimated parameter. The meaning of each column of the table is describen below.

- **Number:** While editing a certain aquifer property or excitation, you have the option to define the extent of an estimated parameter by assigning a unique parameter number to the cells of interest. That unique parameter number corresponds to the **Number** here.
- **Active**: The value of an estimated parameter will only be adjusted if **Active** is checked. Otherwise the user-specified cell value will be used for the simulation. Normally, the total number of active parameters should not exceed 10, although PMWIN allows 150 parameters.
- **Description:** A text describing the estimated parameter can be entered here (optional), for example, “Transmissivity in layer 3”. A maximum of 120 characters is allowed.
- **PARVAL1** is a parameter's initial value. For a fixed parameter, this value remains invariant during the optimization process. For a tied parameter (see PARTRANS below), the ratio of PARVAL1 to the parent parameter's PARVAL1 sets the ratio between these two parameters to be maintained throughout the optimization process. For an adjustable parameter, PARVAL1 is the parameter's starting value which, together with the starting values of all other adjustable parameters, it is successively improved during the optimization process. To enhance optimization efficiency, you should choose an initial parameter value which is close to what you think will be the parameter's optimized value. You should note the following repercussions of choosing an initial parameter value of zero.
  1. Limitation of the parameter adjustment is not possible (see the discussion on RELPARMAX and FACPARMAX) during the first optimization iteration if the starting value of a parameter is zero. Furthermore FACORIG cannot be used to modify the action of RELPARMAX and FACPARMAX for a particular parameter throughout the optimization process, if that parameter's original value is zero.
  2. A relative increment for derivatives calculation cannot be evaluated during the first iteration for a parameter whose initial value is zero. If the parameter belongs to a group for which derivatives are, in fact, calculated as **Relative** (see INCTYP and DERINC below), a non-zero DERINCLB variable must be provided for that group.
  3. If a parameter has an initial value of zero, the parameter can be neither a tied nor a parent parameter as the tied/parent parameter ratio cannot be calculated.
- **PARLBND** and **PARUBND** are a parameter's lower and upper bounds respectively. For adjustable parameters the initial parameter value (PARVAL1) must lie between these two bounds. For fixed and tied parameters, PARLBND and PARUBND are ignored.
- **PARTRANS** controls the parameter transformation. By clicking on a cell of the PARTRANS column, this flag can be set as **None**, **Log-transformed, Tied** or **Fixed**. Use Log-transformed, if you wish that a parameter be log-transformed throughout the

estimation process. A parameter which can become zero or negative in the course of the parameter estimation process must not be log-transformed; hence if a parameter's lower bound is zero or less, PEST will disallow logarithmic transformation for that parameter. Note that by using an appropriate scale and offset, you can ensure that parameters never become negative. Thus if you are estimating the value for a parameter whose domain, as far as the model is concerned, is the interval [-9.99, 10], you can shift this domain to [0.01, 20] for PEST by designating a scale of 1.0 and an offset of -10.0. Similarly if a parameter's model domain is entirely negative, you can make this domain entirely positive for PEST by supplying a scale of -1.0 and an offset of 0.0. See the discussion on the SCALE and OFFSET variables below.

If a parameter is fixed, taking no part in the optimization process, PARTRANS must be specified as **Fixed**. If a parameter is linked to another parameter, this is signified by a PARTRANS value of **Tied**. In the latter case the parameter plays only a limited role in the estimation process. However the parameter to which the tied parameter is linked (this "parent" parameter must be neither fixed nor tied itself) takes an active part in the parameter estimation process; the tied parameter simply "piggy-backs" on the parent parameter, the value of the tied parameter maintaining at all times the same ratio to the parent parameter as the ratio of their initial values. If a parameter is neither fixed nor tied, and is not log-transformed, the parameter transformation variable PARTRANS must be supplied as **None**.

- **PARCHGLIM** is used to designate whether an adjustable parameter is relative-limited or factor-limited (See the discussion on RELPARMAX and FACPARMAX, p. 147). For tied or fixed parameters PARCHGLIM has no significance.
- **PARGP** is the number of the group to which a parameter belongs. Parameter groups are discussed in **Group Definitions** below.
- **PARTIED** is the number of the "parent" parameter to which a parameter is linked. See also PARTRANS.
- **SCALE** and **OFFSET**: Just before a parameter value is written to an input file of MODFLOW, it is multiplied by the real variable SCALE, after which the real variable OFFSET is added. The use of these two variables allows you to redefine the domain of a parameter. Because they operate on the parameter value "at the last moment" before it is sent, they take no part in the estimation process; in fact they can "conceal" from PEST the true value of a parameter as seen by the model, PEST optimizing, instead, the parameter b_p where

$$b_p = (b_m - o)/s \tag{3.51}$$

Here b_p is the parameter optimized by PEST, b_m is the parameter seen by the model, while s and o are the scale and offset values for that parameter respectively. If you wish to leave a parameter unaffected by scale and offset, enter the SCALE as 1.0 and the OFFSET as 0.0.

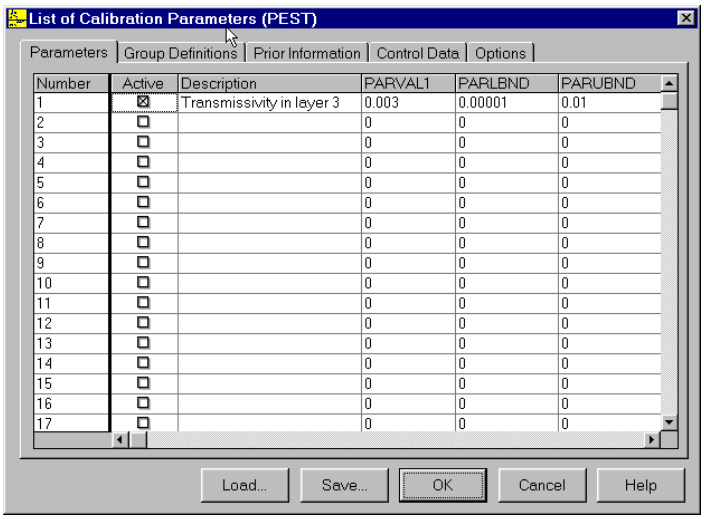


Fig. 3.53 The **List of Calibration Parameters (PEST)** dialog box

- **Group Definitions**

  In PEST, the input variables that define how derivatives are calculated pertain to parameter groups rather than to individual parameters. These input variables are spcified in the Group Definitions tab of the **List of Calibration Parameters (PEST)** dialog box.Thus derivative data does not need to be entered individually for each parameter; however, if you wish, you can define a group for every parameter and set the derivative variables for each parameter separately. In many cases parameters fall neatly into separate groups which can be treated similarly in terms of calculating derivatives.

  - **Number** is the group number. The maximum number of parameter groups is 150.
  - **Description:** A text describing the estimated parameter can be entered here (optional), for example, “Transmissivity Group 1”. A maximum of 120 characters is allowed.
  - **INCTYP** and **DERINC: INCTYP** defines the type of parameter increment (perturbation) used for forward-difference calculation of derivatives with respect to any parameter belonging to the group. INCTYP can be **Relative**, **Absolute** or **Rel_to_max**. If it is **Relative**, the increment is calculated as a fraction of the current value of that parameter; that fraction is specified in DERINC. If INCTYP is **Absolute** the parameter increment is fixed at the value of DERINC and if INCTYP is **Rel_to_max**, the parameter increment is calculated as a fraction of the group member with highest absolute value, that fraction

again being DERINC.

If a group contains members which are fixed and/or tied you should note that the values of these parameters are taken into account when calculating parameter increments using the **Rel_to_max** option. For the **Relative** and **Rel_to_max** options, a DERINC value of 0.01 is often appropriate. However no suggestion for an appropriate DERINC value can be provided for the **Absolute** increment option; the most appropriate increment will depend on the parameter magnitudes.

- **DERINCLB** is the absolute lower limit of parameter increments for all group members. If a parameter increment is calculated as **Relative** or **Rel_to_max**, it may become too low if the parameter becomes very small or, in the case of the **Rel_to_max** option, if the magnitude of the largest parameter in the group becomes very small. A parameter increment becomes "too low" if it does not allow reliable derivatives to be calculated with respect to that parameter because of roundoff errors incurred in the subtraction of nearly equal model-generated observation values. DERINCLB is used to bypass this possibility.

  If you do not wish to place a lower limit on parameter increments in this fashion, you should set DERINCLB to zero. Note that if INCTYP is **Absolute**, DERINCLB is ignored.
- **FORCEN** can be **Always_2**, **Always_3** or **Switch**. It determines how to calculate derivatives for group members. If FORCEN is **Always_2**, derivatives for all parameters belonging to that group will always be calculated using the forward difference method; If FORCEN is **Always_3**, PEST will use central difference method to calculate the devivatives. In this case, twice as many model runs as there are parameters within the group will be required; however the derivatives will be calculated with greater accuracy and this will probably have a beneficial effect on the performance of PEST. If FORCEN is set to **Switch**, derivatives calculations for all adjustable group members will begin using the forward difference method, switching to the central method for the remainder of the estimation process after the relative objective function reduction between successive iterations is less than PHIREDSWH as defined in the **Control Data** (see below).

  Experience has shown that in most instances the most appropriate value for FORCEN is **Switch**. This allows speed to take precedence over accuracy in the early stages of the optimization process when accuracy is not critical to objective function improvement, and accuracy to take precedence over speed later in the process when realization of a (normally smaller) objective function improvement requires that derivatives be calculated with as much accuracy as possible, especially if parameters are highly correlated and the normal matrix thus approaches singularity.
- **DERINCMUL**: If a three-point derivatives calculation is employed, the value of

DERINC is multiplied by DERINCMUL. If you do not wish the parameter increment DERINC to be changed, you must set DERINCMUL to a value of 1.0. Alternatively, if for some reason you wish the increment to be reduced if three-point derivatives calculation is employed, you should provide DERINCMUL with a value of less than 1.0. Experience shows that a value between 1.0 and 2.0 is usually satisfactory.

- **DERMTHD** defines the variant of the central (ie. three-point) method used for derivatives calculation and is used only when FORCEN is **Always_3** or **Switch**. PEST provides three vaiants: **Parabolic**, **Best_fit** or **Outside_pts**. Refer to the manual of PEST for details about these methods.

- **Prior Information**

It often happens that we have some information concerning the parameters that we wish to optimize, and that we obtained this information independently of the current experiment. This information may be in the form of other unrelated estimates of some or all of the parameters, or of relationships between parameters. It is often useful to include this information in the parameter estimation process because it may lend stability to the process.

To define a prior information, first check the **Active** flag in the **Prior Information** tab, then enter the prior information equation in the **Prior Information** column. The syntax of a prior information equation is

PIFAC * PARNME + PIFAC * log(PARNME) .... = PIVAL WEIGHT (3.52)

To the left of the "=" sign there are one or more combinations of a factor (PIFAC) plus parameter name (PARNME), with a "log" prefix to the parameter name if appropriate. PIFAC and PARNME are separated by a "*" character (which must be separated from PIFAC and PARNME by at least one space) signifying multiplication. All parameters referenced in a prior information equation must be adjustable parameters; i.e., you must not include any fixed or tied parameters in a prior information equation. Furthermore, any particular parameter can be referenced only once in any one prior information equation. If a parameter is log-transformed, you must provide prior information pertinent to the log (to base 10) of that parameter. The parameter name must be placed in brackets and preceded by "log" (note that there is no space between "log" and the following opening bracket). Care must be used here, because PMWIN does not check the prior information equation. However, you can use the program PESTCHEK (Doherty et al., 1994) included in PMWIN to check the PEST data.

To the right of the "=" sign of each prior information equation are two real variables PIVAL and WEIGHT. The former is the value of the right hand side of the prior information

equation. The latter is the weight pertaining to the article of prior information in the parameter estimation process. The weight should be inversely proportional to the standard deviation of the prior information value (PIVAL); it can be zero if you wish, but not be negative. The following lines show some examples, refer to Doherty et al. (1994) for more details on the prior information. In PMWIN, the parameter name of the first parameter is P1. The parameter name of the second parameter is P2 and so on.

```
1.0 * log(P1) + 1.2 * log(P2) = -5.6 1.0
1.0 * P1 + 1.455 * P2 - 3.98 * P3 + 2.123 * P4 = 1.03E-3 2.00
2.12 * P3 + 3.2 * P6 = 1.344 2.20
```

- **Control Data**

  The control data are used to set internal array dimensions of PEST and tune the optimization algorithm to the problem at hand. The items of the control data are described in detail below. When in doubt, you should use the default values given by PMWIN.

  - **RLAMBDA1** is the initial Marquardt lambda. PEST attempts parameter improvement using a number of different Marquardt lambdas during any one optimization iteration. In the course of the overall parameter estimation process, the Marquardt lambda generally gets smaller. An initial value of 1.0 to 10.0 is appropriate for many models, though if PEST complains that the normal matrix is not positive definite, you will need to provide a higher initial Marquardt lambda. For high values of the Marquardt parameter (and hence of the Marquardt lambda) the parameter estimation process approximates the gradient method of optimization. While the latter method is inefficient and slow if used for the entire optimization process, it often helps in getting the process started, especially if initial parameter estimates are poor. PEST reduces lambda if it can. However if the normal matrix is not positive definite or if a reduction in lambda does not lower the objective function, PEST has no choice but to increase lambda.
  - **RLAMFAC** is the factor by which the Marquardt lambda is adjusted. RLAMFAC must be greater than 1.0. When PEST reduces lambda it divides by RLAMFAC; when it increases lambda it multiplies by RLAMFAC.
  - **PHIRATSUF** is the first criterion for moving to the next optimization iteration. During any one optimization iteration, PEST tries lots of parameter sets and will consider that the goal of the iteration has been achieved if

$$\frac{\Phi_i}{\Phi_{i-1}} \leq PHIRATSUF \qquad (3.53)$$

where ϕ_{i-1} is the lowest objective function calculated for optimization iteration i-1 (and hence the starting value for the i-th optimization iteration) and ϕ_i is the objective function corresponding to a parameter set during optimization iteration i.

A value of 0.3 is often appropriate for PHIRATSUF. If it is set too low, model runs may be wasted in search of an objective function reduction which it is not possible to achieve. If it is set too high, PEST may not be given the opportunity of refining lambda in order that its value continues to be optimal as the parameter estimation process progresses.

- **PHIREDLAM** is the second criterion for moving to the next optimization iteration. If the first criterion PHIRATSUF cannot be achieved during an optimization iteration, PEST uses PHIREDLAM to decide when it should move on to the next iteration. If the relative reduction in the objective function between the use of two consecutive parameter sets is less than PHIREDLAM, PEST moves to the next iteration (i+1). That is

$$\frac{(\Phi_i^{j-1} - \Phi_i^j)}{\Phi_i^{j-1}} \leq PHIREDLAM \qquad (3.54)$$

where Φ_i^j is the objective function value calculated during the i-th iteration using the j-th trial parameter set.

A suitable value for PHIREDLAM is often around 0.01. If it is set too large, the criterion for moving on to the next optimization iteration is too easily met and PEST is not given the opportunity of adjusting lambda to its optimal value for that particular stage of the parameter estimation process. On the other hand if PHIREDLAM is set too low, PEST will test too many Marquardt lambdas (too many parameter sets) on each iteration step when it would be better off starting a new iteration.

- **NUMLAM** is the maximum number of lambdas (parameter sets) that PEST can test during any one optimization iteration. It should normally be set between 5 and 10. For cases where parameters are being adjusted near their upper or lower limits, and for which some parameters are consequently being frozen (thus reducing the dimension of the problem in parameter space) experience has shown that a value closer to 10 may be more appropriate than one closer to 5.
- **RELPARMAX and FACPARMAX** are used to limit parameter adjustments. RELPARMAX is the maximum relative change that a parameter is allowed to undergo between iterations, whereas FACPARMAX is the maximum factor change that a parameter is allowed to undergo. A parameter is denoted as either relative-limited or factor-limited through PARCHGLIM (see p. 142).

If a parameter b is **relative-limited**, The relative change between optimization iterations i-1 and i is defined as

$$\frac{(b_{i-1} - b_i)}{b_{i-1}} \tag{3.55}$$

The absolute value of this relative change must be less than RELPARMAX. If a parameter upgrade vector is calculated such that the relative adjustment for one or more relative-limited parameters is greater than RELPARMAX, the magnitude of the upgrade vector is reduced such that this no longer occurs.

If parameter b is **factor-limited**, the factor change between optimization iterations i-1 and i is defined as

$$\begin{aligned} &b_{i-1}/b_i && \text{if } |b_{i-1}| > |b_i|, \quad \text{or} \\ &b_i/b_{i-1} && \text{if } |b_i| > |b_{i-1}| \end{aligned} \tag{3.56}$$

This factor change must be less than FACPARMAX. If a parameter upgrade vector is calculated such that the factor adjustment for one or more factor-limited parameters is greater than FACPARMAX, the magnitude of the upgrade vector is reduced such that this no longer occurs. It is important to note that a factor-limit will not allow a parameter to change sign. If a parameter must be free to change sign during an optimization process, it must be relative-limited; furthermore RELPARMAX must be set at greater than unity or the change of sign will be impossible. Similarly, if a parameter's upper or lower limit is zero, it cannot be factor-limited and RELPARMAX must be at least unity.

Suitable values for RELPARMAX and FACPARMAX can vary enormously from case to case. If you are unsure of how to set these parameters, a value of 5 for each of them is often suitable. For highly non-linear problems, these values are best set low. If they are set too low, however, the estimation process can be very slow. An inspection of the PEST run record (by pressing the ESC key) will often show whether you have set these values too low, for PEST records the maximum parameter factor and relative changes are recorded on this file at the end of each optimization iteration. If these changes are always at their upper limits and the estimation process is showing no signs of instability, it is quite possible that RELPARMAX and/or FACPARMAX are too low and could be increased.

Note that FACPARMAX can never be less than 1; RELPARMAX can be less than 1 as long as no parameter's upper and lower bounds are of opposite sign. (If necessary, use OFFSET to shift the parameter domain so that it does not include zero.)

- **FACORIG** is a criterion for modifying RELPARMAX and FACPARMAX. If, in the course of an estimation process, the absolute value of a parameter falls below the product

of FACORIG and its original value, then the product is substituted for the denominators of eq. 3.55 or eq. 3.56 to prevent the denominators becoming zero or too small. FACORIG is not used to adjust limits for log-transformed parameters. FACORIG must be greater than zero. A value of 0.001 is often adequate.

- **PHIREDSWH** is a criterion for switching the calculation method of derivatives between the forward finite difference method and the central finite difference method. If, for the i-th iteration the relative reduction in the objective function between successive optimization iterations is less than PHIREDSWH, PEST will switch to three-point derivatives calculation for those parameter groups with FORCEN = **Switch.** The relative reduction in the objective function is defined by $[(\phi_{i-1} - \phi_i) / \phi_{i-1}]$, where ϕ_i is the objective function calculated on the basis of the upgraded parameter set determined in the i-th iteration.

  A value of 0.1 is often suitable for PHIREDSWH. If it is set too high, PEST may make the switch to three-point derivatives calculation too early. The result will be that more model runs will be required than are really needed at that stage of the estimation process. If PHIREDSWH is set too low, PEST may waste an optimization iteration or two in lowering the objective function to a smaller extent than would have been possible, if it had made an earlier switch to central derivatives calculation.

  Note that PHIREDSWH should be set considerably higher than PHIREDSTP (see below) which sets one of the termination criteria on the basis of the relative objective function reduction between optimization iterations.
- **NOPTMAX** is the maximum number of optimization iterations. A value of 20 to 30 is often adequate. If you want to ensure that PEST termination is triggered by other criteria, more indicative of parameter convergence to an optimal set or of the futility of further processing, you should set this variable very high.
- **PHIREDSTP** and **NPHISTP** are convergence criteria. For many cases 0.01 and 3 are suitable values for PHIREDSTP and NPHISTP respectively.

  If, in the course of the parameter estimation process, there have been NPHISTP optimization iterations for which

$$\frac{(\Phi_i - \Phi_{min})}{\Phi_i} \leq PHIREDSTP \qquad (3.57)$$

  (ϕ_i being the objective function value at the end of the i-th optimization iteration and ϕ_{min} being the lowest objective function achieved to date), PEST will end the optimization process.
- **NPHINORED** is the first termination criterion. A value of 3 is often suitable. If PEST has

failed to lower the objective function over NPHINORED successive iterations, the program stops.

- **RELPARSTP** and **NRELPAR** represent the second termination criterion. If the magnitude of the maximum relative parameter change between optimization iterations is less than RELPARSTP over NRELPAR successive iterations, the program stops. The relative parameter change between optimization iterations for any parameter is calculated using equation 3.55. For many cases, a value of 0.01 for RELPARSTP and a value of 3 for NRELPAR is adequate.

- **Options:**

When the optimization process is complete, one of the termination criteria having been met (or perhaps another termination criterion such as zero objective function or zero objective function gradient, for which no user-supplied settings are required), PEST writes some information concerning the optimized parameter set to its run record file PESTCTL.REC. This file is saved in the data directory of your model. It tabulates the optimal values and the 95% confidence intervals pertaining to all adjustable parameters. It also tabulates the model-calculated values based on these parameters, together with the residuals, i.e., the differences between measured and model-calculated values. If you wish, PEST will write the **parameter covariance matrix**, the **parameter correlation coefficient matrix** and the **matrix of normalised eigenvectors** of the covariance matrix to the run record file PESTCTL.REC.

If the option **Save data for a possible restart** is checked, PEST will dump the contents of many of its data arrays to a binary file at the beginning of each optimization iteration; this allows PEST to be restarted later if execution is prematurely terminated. If subsequent PEST execution is initiated using the "/r" command line switch (see the PEST manual for details), it will recommence execution at the beginning of the iteration during which it was interrupted.

If the option **Include decimal point even if redundant** is not checked, PEST will omit the decimal point from parameter values on model input files if the decimal point is redundant, thus making room for the use of one extra significant figure. If this option is checked, PEST will ensure that the decimal point is always present.

PEST (Inverse Modeling) ▸ Run...

To start a model calibration with PEST, select this menu item. The available settings of the **Run PEST** dialog box (Fig. 3.54) are described below.

- **Modflow Version** and **Modflow Program:** Several variants of MODFLOW are included in PMWIN. PMWIN automatically installs the executables of these variants. Their full paths and filenames are given in table 3.4. If you want to use a compiled version located in an other position, click the **open file** button  and select the desired code from a dialog box. The **User's own** version must be selected, if you want to use your own version of MODFLOW. Refer to Appendix 5 for how to configure PMWIN to run with your own MODFLOW.
- **PEST Program**: There are four variants of PEST, which are named PESTLITE, PESTLM, PESTSW and PESTEM. PESTLITE (included in PMWIN) is an educational version of PESTLM and is restricted to 4 parameters and 80 observations. Use of the other three variants is identical; however they each use your machine's memory in a different way. PESTLM is the most basic of the three. It uses conventional DOS memory (limited to 640k), staying resident in this memory when it runs MODFLOW. PESTSW is identical to PESTLM except it vacates the conventional memory as it calls MODFLOW. PESTEM uses your machine's extended memory and executes faster, as it was compiled with a 32-bit compiler. However, an unsolved memory problem will occur, if you run PESTEM within Windows. The problem is probably caused by the operating system or the 32-bit compiler. Fortunately, PESTLM is sufficient for most groundwater problems. **You should use PESTLM unless you have other problems with the conventional memory.**
- **The File Table:** PMWIN uses the user-specified data to generate input files of MODFLOW and PEST. **Description** gives the name of the packages used in the flow model. The path and name of the input file are shown in **Destination File**. PMWIN generates an input file only if the corresponding **Generate** flag is checked. You may click on a flag to check or uncheck it. Normally, you do not need to worry about these flags, as PMWIN will care about the settings.
- **Options**:
  - **Regenerate all input files for MODFLOW and PEST:** You should check this option, if the input files have been deleted or overwritten by other programs.
  - **Generate input files only, don't start PEST:** Check this option, if you do not want to run PEST. You can start the simulation at a later time by executing the batch file PEST.BAT.
  - **Perform PESTCHEK prior to running PEST:** PESTCHEK reads the PEST input files

generated by PMWIN, making sure that every item is consistent with every other item and writes errors to the file PEST.CHK. It is recommended to use PESTCHEK, as PMWIN and PEST do not carry out consistency checks of all user-specified control data and parameters.

- **Check the model data:** Before creating data files for MODFLOW, PMWIN will check the geometry of the model and the consistency of the model data given in table 3.5, if this option is checked. The errors (if any) are saved in the file CHECK.LST located in the same folder as your model data.

▸ **OK**: Click **OK** to start the generation of the MODFLOW and PEST input files. In addition, PMWIN generates two batch files PEST.BAT and MODELRUN.BAT in your model folder. When all necessary files are generated, PMWIN automatically runs PEST.BAT in a DOS-window. The other batch file MODELRUN.BAT will be called by PEST. After completing the parameter estimation process, PEST prints the optimized parameter values to the run record file PESTCTL.REC in your model folder and writes the optimized parameter values to the corresponding input files of MODFLOW (BCF.DAT, WEL.DAT,... , etc.). The simulation results of MODFLOW are updated by using these parameter values.

Note that PMWIN does not retrieve the optimized parameter values into the data matrices. Your (PMWIN) model data will not be modified in any way. This provides more security for the model data, because an automatic calibration process does not necessarily lead to success. If you want to operate on a calibrated model, you can **import** the calibrated MODFLOW model by choosing **Convert Model...** from the **File** menu.

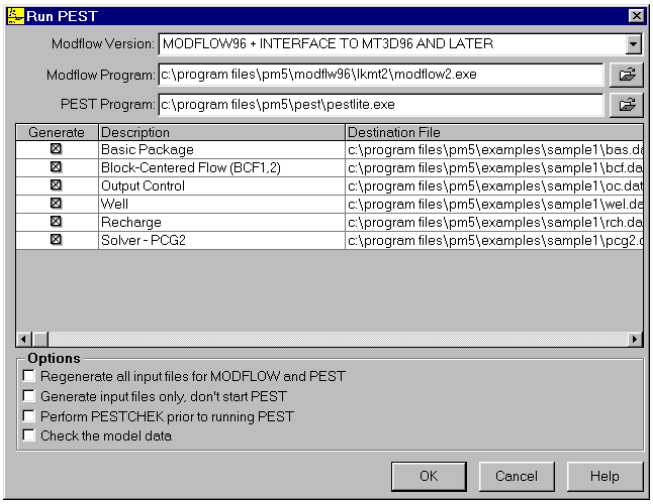


Fig. 3.54 The **Run PEST** dialog box

3.6.6 UCODE (Inverse Modeling)

This menu provides an interface between PMWIN, the flow model MODFLOW and the inverse model UCODE. The use of this interface is very similar to that of PEST. The adjustable parameters and/or excitations are given in Table 3.7. During a calibration process, UCODE searches for a parameter set for which the sum of squared deviations between model-calculated and measurement values at the observation boreholes is reduced to a minimum. The coordinates of the observation boreholes and measurement values are given in **Parameters ▸ Boreholes and Observations**. A simultaneous fit of highly correlated parameters, for example transmissivities and recharge for given head observations, is of little value in steady-state problems due to the non-uniqueness of such a fit.

▸ **To define an estimated parameter**

1. From the **Parameters** or **Models▸Modflow** menu, select a parameter or a package, for example *Horizontal Hydraulic Conductivity* or *Well*.
2. Assign a unique parameter number to cells within an area where the parameter value will be estimated. If you intend to calibrate the pumping rate of wells or the conductance of head-dependent cells (e.g., drain, general head-boundary, river or stream cells), you must also assign a non-zero pumping rate or conductance to those cells. Pumping rate or conductance values will not be adjusted, if the user-specifed values are equal to zero.
3. Use the **List of Calibration Parameters (UCODE)** dialog box to activate the estimated parameter and to specify the necessary values.

Note that for layers of type **0:confined** and **2:confined/unconfined (transmissivity=const.)**, MODFLOW reads transmissvity (instead of hydraulic conductivity) from the model data file. Consequently, you are actually calibrating the transmissivity value as an estimated parameter defined within horizontal hydraulic conductivity. For multi-layer models, MODFLOW requires vertical leakance (instead of vertical hydraulic conductivity, which is used by PMWIN to calculate the vertical leakance for MODFLOW). Due to this fact, automatic fit of vertical hydraulic conductivity cannot be done without modifying the inverse model or MODFLOW. So, if you assign an estimated parameter within vertical hydraulic conductivity, you should keep in mind that you are actually calibrating the vertical leakance between two layers (the layer of the estimated parameter and the underlying layer).

UCODE (Inverse Modeling) ▸ Parameter List...

The required inputs and options for the PMWIN/MODFLOW/UCODE interface are specified in the **List of Calibration Parameters (UCODE)** dialog box (Fig. 3.55). The options are grouped under four tabs described below.

- **Parameters:** The table gives an overview of the initial values and properties of each estimated parameter. The meaning of each column of the table is describen below.
  - **Number:** While editing a certain aquifer property or excitation, you have the option to define the extent of an estimated parameter by assigning a unique parameter number to the cells of interest. That unique parameter number corresponds to the **Number** here.
  - **Active**: The value of an estimated parameter will only be adjusted if **Active** is checked. Otherwise the user-specified cell value will be used for the simulation. Normally, the total number of active parameters should not exceed 10, although PMWIN allows 150 parameters.
  - **Description:** A text describing the estimated parameter can be entered here (optional), for example, “Transmissivity in layer 3”. A maximum of 120 characters is allowed.
  - **Start-value** is a parameter's initial value.
  - **Minimum** and **Maximum** are the reasonable minimum and maximum values for the parameter. The values are used solely to determine how the final optimized value of this parameter compares to a reasonable range of values. Do not specify the “log” of log-transformed parameters; they are calculated by the program.
  - **Log-transform:** Check this flag to log-transform the parameter. Typically log-transformed parameters are those for which negative values are not reasonable (for example hydraulic conductivity).

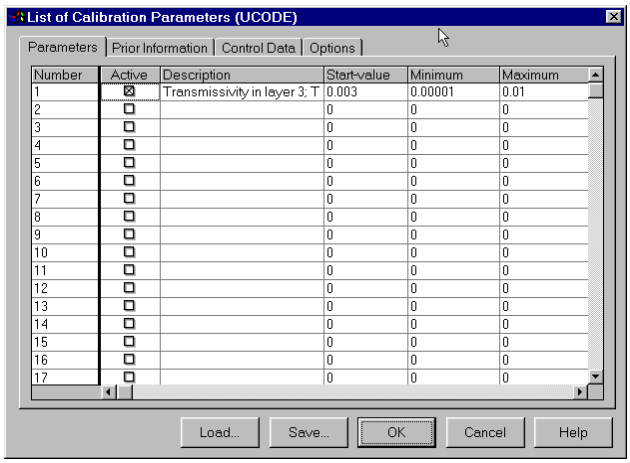


Fig. 3.55 The **List of Calibration Parameters (UCODE)** dialog box

- **Prior Information**:
  Similar to PEST, prior information can be defined in the UCODE modeling environment. To define a prior information, first check the **Active** flag in the **Prior Information** tab, then enter the prior information equation in the **Prior Information** column. The syntax of a prior information line is

  P EQUATION stat STAT flag STAT-FLAG plot PLOT-SYMBOL (3.58)

  where EUQATION is defined by eq. 3.59.

  PVALUE = C1 x P1 & C2 x P2 ..... (3.59)

  The components of eq. 3.58 and 3.59 need to be separater by one space. The components are defined as follows.
  - P is the code indicating that a prior information line follows.
  - PVALUE: The prior information value. Specify the decimal value, even for a log-transformed parameter.
  - C1, C2: Coefficients with values as specified by the user.
  - x: Indicates multiplication. Needs to be preceded and followed by one blank space.
  - P1, P2: Parameter names. The parameter name of the first parameter is P1. The parameter name of the second parameter is P2 and so on (see examples below).
  - &: Indicates that the preceding and following products are to be summed; thus, it performs like a +.
  - stat is a label followed by STAT.
  - STAT is a statistic value used to calculate the weight for the prior information. For log-transformed parameters, specify the log-transformed statistic, even though PVALUE is a decimal value.
  - flag is a lable followed by STAT-FLAG.
  - STAT-FLAG is a flag indicating whether STAT is a variance (STAT-FLAG=0), standard deviation (STAT-FLAG=1) or coefficient of variation (STAT-FLAG=2).
  - plot is a label followed by PLOT-SYMBOL.
  - PLOT-SYMBOL is an integer printed in the UCODE output file (UCODE._ot) used for graphical analyses. Different values for plot-symbol can be used to indicate different types of observations so that they can be differentiated with a unique symbol on a graph. The utility of PLOT-SYMBOL will depend on the graphical software being used.

  The following lines show some examples, refer to Hill (1998) and Poeter and Hill (1998) for

more details about the use of the prior information.

```
P 10 = 0.5 x P1 & 0.5 x P2 stat 0.2 flag 2 plot 4
P 1.03E-3 = 1.0 x P1 & 1.45 x P2 & -3.9 x P3 & 2.123 x P4 stat 2.0 flag 2 plot 3
P 1.344 = 2.12 x P3 & 3.2 x P6 stat 2.2 flag 2 plot 1
```

- **Control Data**

  The control data are used to control the sensitivity and regression calculations and define the inversion algorithm. The items of the control data (Fig. 3.56) are described below.

  - **Convergence criterion (TOL)**: When parameter values change less than this fractional amount between regression iterations, parameter estimation converges (0.01 is recommended).
  - **Convergence criterion (SOSR)**: When the sum-of-squared, weighted residuals changes less than this fractional amount over three regression iterations, parameter estimation converges. Ideally, for the final results convergence is achieved by satisfying the TOL criterion so that SOSR can be equal to 0.0 (in which case SOSR is not used as a convergence criteria). Values of SOSR of 0.01 and even 0.1 can be useful, however, in the early stages of model calibration because it stops the regression when it is not progressing.
  - **Maximum number of regression iterations (MAX-ITER)** is self-explanatory. Starting with twice the number of parameters is recommended.
  - **Maximum fractional parameter change (MAX-CHANGE)** is the maximum fractional change of a parameter value allowed in one regression iteration. For example, if MAX-CHANGE = 2.0, a parameter value of 1.0 will not be allowed to change by more than 2.0 (MAX-CHANGE times the parameter value). Consequently, the new value will be between -1.0 and 3.0. A parameter value of 2.0 will not be allowed to change more than a value of 4.0 (again, MAX-CHANGE times the parameter value), and the new value will be between -2.0 and 6.0). This maximum change is applied to the physical parameter value, not its log transformed value. Exceptions are discussed in Hill (1998, Appendix B). MAX-CHANGE = 2.0 is common, but smaller values may help an oscillating regression to converge.
  - **Differencing method** controls the method used to calculate sensitivities during the parameter-estimation iterations. Starting with the forward differencing method is recommended.
  - **Apply quasi-Newton update when sum-of-squared, weighted residuals changes less than 0.01 over three regression iteration.** According to Hill (1998), applying the quasi-

Newton update may facilitate convergence of highly nonlinear problems.

- **Options**
  - **Print residuals and sensitivities for intermediate iterations:** When it is checked, the residuals and sensitivities will be printed (saved) for intermediate iterations in the output file UCODE._ot.
  - **Scale Sensitivities:** Controls the scaling applied to the printed sensitivities. Four options are available.
    1. **No scaling:** unscaled sensitivities are printed.
    2. **Dimensionless scaled sensitivities are printed**: Sensitivities are scaled by the parameter value times the square-root of the weight, resulting in dimensionless numbers. Composite scaled sensitivities also are printed.
    3. **One-percent scaled sensitivities are printed:** Sensitivities are scaled by the parameter value divided by 100, resulting in numbers with the dimensions of the observations.
    4. **Both dimensionless and one-percent scaled sensitivities are printed.**

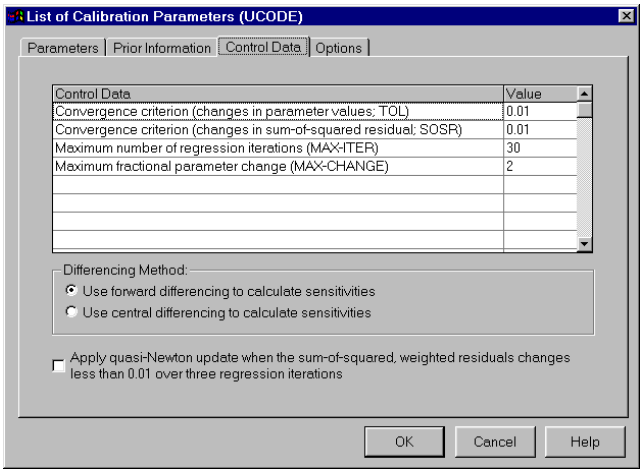


Fig. 3.56 Control data of UCODE

UCODE (Inverse Modeling) ▸ Run...

To start a model calibration with UCODE, select this menu item. The available settings of the **Run UCODE** dialog box (Fig. 3.57) are described below.

- **Modflow Version** and **Modflow Program:** Several variants of MODFLOW are included in PMWIN. PMWIN automatically installs the executables of these variants. Their full paths and filenames are given in table 3.4. If you want to use a compiled version located in an other

position, click the **open file** button  and select the desired code from a dialog box. The **User's own** version must be selected, if you want to use your own version of MODFLOW. Refer to Appendix 5 for how to configure PMWIN to run with your own MODFLOW.

- **Inverse Code** is the name of the nonlinear regression executable (*mrdrive.exe*, as distributed). If another inversion algorithm is used, its full path and file name need to be specified here.
- **The File Table:** PMWIN uses the user-specified data to generate input files of MODFLOW and UCODE. **Description** gives the name of the packages used in the flow model. The path and name of the input file are shown in **Destination File**. PMWIN generates an input file only if the corresponding **Generate** flag is checked. You may click on a flag to check or uncheck it. Normally, you do not need to worry about these flags, as PMWIN will take care of the settings.
- **Options**:
  - **Regenerate all input files for MODFLOW and UCODE:** You should check this option, if the input files have been deleted or overwritten by other programs.
  - **Generate input files only, don't start UCODE:** Check this option, if you do not want to run UCODE. You can start the simulation at a later time by executing the batch file UCODE.BAT.
  - **Check the model data:** Before creating data files for MODFLOW and UCODE, PMWIN will check the geometry of the model and the consistency of the model data given in table 3.5, if this option is checked. The errors (if any) are saved in the file CHECK.LST located in the same folder as your model data.
- **OK**: Click **OK** to start the generation of the MODFLOW and UCODE input files. In addition, PMWIN generates two batch files UCODE.BAT and UCODE1.BAT in your model folder. When all necessary files are generated, PMWIN automatically runs UCODE.BAT in a DOS-window. UCODE1.BAT will be called by the inversion code. After completing the parameter estimation process, UCODE prints the optimized parameter values to the run record file *UCODE._ot* in your model folder and automatically writes the optimized parameter values to the input files of MODFLOW (BCF.DAT, WEL.DAT,... , etc.). The simulation results of MODFLOW are updated by using these parameter values.

  Note that PMWIN does not retrieve the optimized parameter values into the data matrices. Your (PMWIN) model data will not be modified in any way. This provides more security for the model data, because an automatic calibration process does not necessarily lead to success. If you want to operate on a calibrated model, you can **import** the calibrated MODFLOW model by choosing **Convert Model...** from the **File** menu.

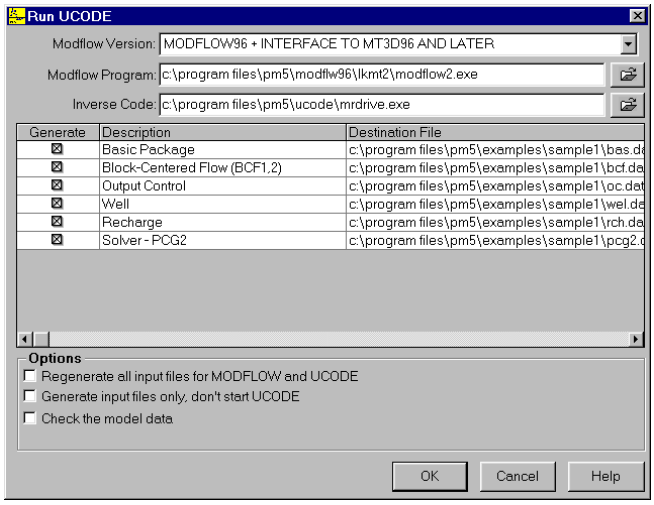


Fig. 3.57 The **Run UCODE** dialog box

3.6.7 PMPATH (Pathlines and Contours)

Select this menu to call the particle tracking model PMPATH, which runs independently from PMWIN. Refer to Chapter 4 for details about PMPATH.

Note that the first time you call PMPATH, it will automatically load the model currently used by PMWIN. If you have subsequently modified model data and performed a flow simulation, you must reload the modified model into PMPATH to ensure that it can recognize the modifications.

3.7 The Tools menu

PMWIN provides several modeling tools, including Digitizer, Field Interpolator, Field Generator, Results Extractor, Water Budget Calculator, and Graph Viewer. Refer to Chapter 5 for details.

3.8 The Value menu

The **Value** menu appears only in the **Data Editor**. The menu items are described below.

Matrix...

Use the **Browse Matrix** dialog box (Fig. 3. 58) to examine cell values. The spreadsheet displays a series of columns and rows, which corresponds to the columns and rows of the finite-difference grid. The cell data are shown in the spreadsheet. If you are editing a particular package, in which a cell has more than one value (for example, the River package requires three values for each cell), you can select the parameter type from the **Parameter** drop-down box. The **Column Width** drop-down box is used to change the appearance width of the columns of the spreadsheet. You may edit the cell data within the **Browse Matrix** dialog box. You may also assign a value to a group of cells by using the mouse to mark the cells and then enter the desired value.

You may save the cell data by clicking the **Save...** button and specifying the file name and the file type in a **Save Matrix As...** dialog box. There are four file types, *ASCII Matrix (Wrap form), ASCII Matrix*, *SURFER files* and *SURFER files (real-world).* An *ASCII Matrix* file may be loaded into the spreadsheet at a later time. The format of the ASCII matrix file is described in Appendix 2. A SURFER file has three columns containing the (x, y) coordinates and the value of each cell. If the file type is *SURFER files*, the origin of the coordinate system for saving the file is set at the lower-left corner of the model grid. If the file type is *SURFER files (real-world)*, the real-world coordinates of each cell will be saved. The real-world coordinate system is defined by **Options ▸ Environment.**

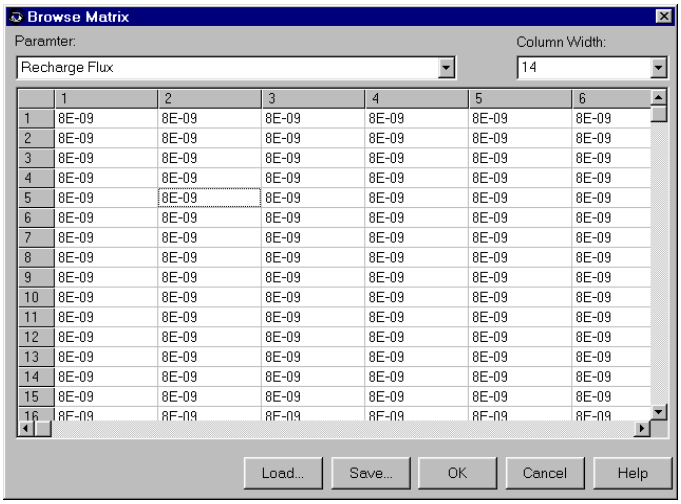


Fig. 3.58 The **Browse Matrix** dialog box

▸ **To load an ASCII Matrix or a SURFER GRD file**

1. Click the **Load...** button.
   The **Load Matrix** dialog box appears (Fig. 3.59)
2. Click  and select a file type (i.e., ASCII Matrix or SURFER GRD) and a file from an **Open File** dialog box.
3. Specify the starting position.
   As shown in Fig. 3.60, the starting position indicates the column and row at which a matrix will be loaded. Numbers of rows and columns of the loaded matrix need not to be identical to those of the finite-difference grid. This allows you to replace only part of the cell data by the matrix. For example, you can use the **Field Generator** to generate a matrix with heterogeneously distributed data from statistic parameters and load it into the grid as a subregion.
4. Select an option from the **Options** group. Just before a loaded matrix is put to the spreadsheet, its values will be modified according to the following options.

   Replace: The cell data in the spreadsheet are replaced by those of the ASCII Matrix.
   Add: The cell values of the ASCII Matrix are added to those of the spreadsheet.
   Subtract: The cell data in the spreadsheet are subtracted from those of the loaded matrix.
   Multiply: The cell data in the spreadsheet are multiplied by those of the loaded matrix.
   Divide: The cell data in the spreadsheet are divided by those of the loaded matrix. If a cell value of the loaded matrix is equal to zero, the corresponding cell value in the spreadsheet remains unchanged.

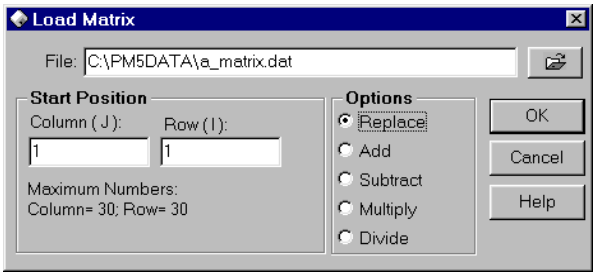


Fig. 3.59 The **Load Matrix** dialog box

Notes

1. **Because of the nature of SURFER, a SURFER GRD file may only be used with regularly spaced model grids. Consider to use the Field Interpolator (see Chapter 5), if your model grid is irregularly spaced.**
2. **PMWIN only accepts SURFER GRD files, which are saved in ASCII.**

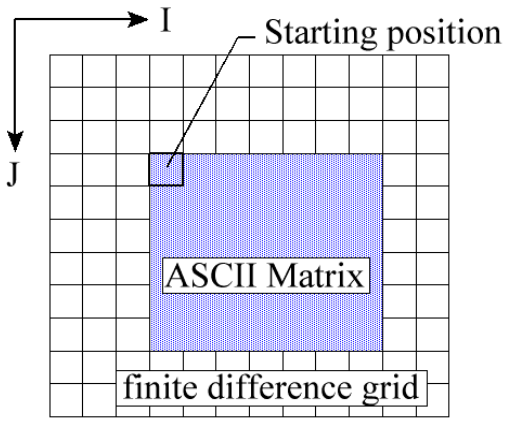


Fig. 3.60 The starting position of a loaded ASCII matrix.

Reset Matrix...

Using Reset Matrix... you can specify a value in a **Reset Matrix** dialog box. The value will be assigned to all finite-difference cells. If you are editing a particular package, in which a cell has more than one value (for example the River package), all values in the dialog box will be assigned to all cells.

Zones

The Zones menu allows you to save or load the zones in or from a Zone file. All zones in the layer being edited can be deleted by selecting **Zones▸Delete All**. Using Zone files, you can transfer zonation information between parameters or between models with different grid configuration. The format of the Zone file is given in Appendix 2.

Points

The **Points** menu appears only in the **Digitizer**. Refer to Chapter 5 for details about the Digitizer and the **Points** menu.

Search and Modify

Use the **Search and Modify** dialog box (Fig. 3.61), if you want to automatically modify part of the cell data or if you want to create solid fill plots based on the cell data. The items of the dialog box are described below:

- **The Trace Table**: You define a search range and its attributes in an active row of the table. A row is active when the **Active** flag is checked. The search range is given by the minimum (lower limit) and the maximum (upper limit). The color in the **Color** column will be assigned to the finite-difference cells that have a value located within the search range.

  You can automatically assign regularly-spaced search ranges to each active row by clicking on one of the headers **Minimim** or **Maximum**, then enter a minimum and a maximum value to a **Search Level** dialog box.

  The colors can be automatically assigned so you will get a gradational change from one color to another. To do this, click the header **Color** of the table and assign a minimum color and a maximum color to a **Color Spectrum** dialog box. To change the color individually, click on the colored cell (a button appears), then click on the button and select a color from a **Color** dialog box.

  According to the user-specified value (in the **Value** column) and the operation option (in the **Options** column), you can easily modify the cell values. The available operations are listed below:

  - **Display Only**: No operation takes place.
  - **Replace**: The cell values are replaced by the user-specified value.
  - **Add**: The user-specified value is added to the cell values.
  - **Multiply:** The cell values are multiplied by the user-specified value.
- **Parameter drop-down box**: For particular packages, in which a cell has more than one value (e.g., the River package of MODFLOW), this drop-down box contains the available parameter type(s). Choose the parameter type for which the *Search and Modify* operation will apply.
- **Ignore Inactive Cells**: If it is checked, the *Search and Modify* operation will only be applied to active cells.
- **Maps**: You may display background maps (DXF or Line Map) by using the Maps Options dialog box. See section 3.9 for details.
- **Save...** and **Load...**: The entries in the **Trace Table** can be saved or loaded in *trace* files. The format of the trace file is given in Appendix 2.

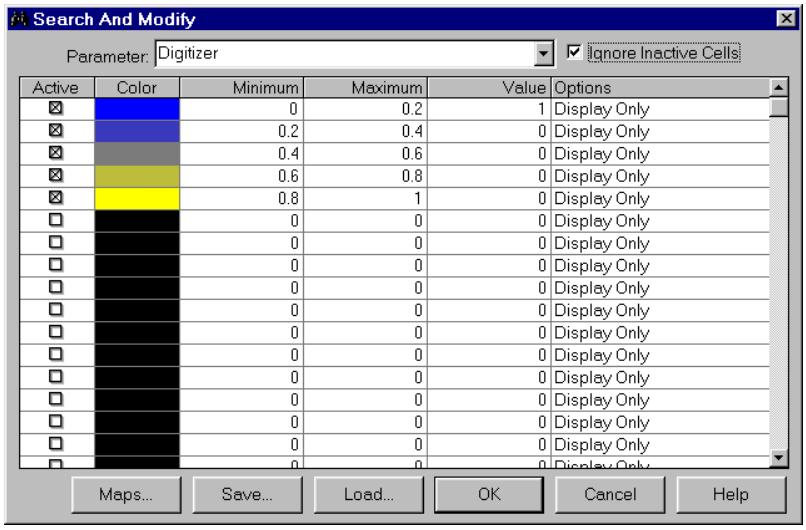


Fig. 3.61 The **Search and Modify** dialog box

Result Extractor...

You may use this menu item to call the Result Extractor. Refer to Chapter 5 for details about the use of this modeling tool.

Boreholes and Observations...

You may use this menu item to open the Boreholes and Observations dialog box. Refer to section 3.5 for details about this dialog box.

3.9 The Options menu

There are four menu items in the **Options** menu; namely **Environment**, **Maps**, **Display Mode** and **Input Method**. The use of the menu items **Environment** and **Maps** is described below. Refer to section 3.2 for the description of the display modes and input methods.

Environment...

The **Environment Options** dialog box allows you to configure the coordinate system and modify appearance of the model grid. Available settings are grouped under three tabs: **Appearance**,

Coordinate System and **Contours**. The checkbox **Display zones in the cell-by-cell mode** is used to force PMWIN to display the user-specified zones in the cell-by-cell input mode.

- **Appearance** (Fig. 3.62) allows you to change the visibility and appearance color of each simulated component. A simulated component is visible if the corresponding **Visibility** checkbox is checked. To select a new color, click on the colored cell (a button appears), then click on the button and select a color from a **Color** dialog box.

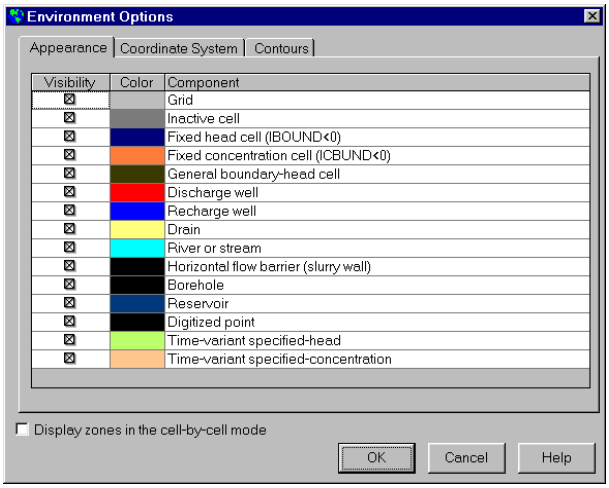


Fig. 3.62 The **Appearance** tab of the **Environment Options** dialog box

- **Coordinate System** is used to define the extent and location of the area of interest (the worksheet) and to define location and orientation of the model grid.

  As illustrated in Fig. 3.63, the worksheet is a "window" to the real-world, your model grid is placed within the worksheet. The extent and location of the worksheet are defined by specifying the (real-world) coordinates of its lower-left and upper-right corners; i.e., by the coordinates (X_1, Y_1) and (X_2, Y_2) as shown in Fig. 3.63 and Fig. 3.64. The location and orientation of the model grid are defined by the coordinates (X_0, Y_0) of its left-upper corner and a rotation angle. The rotation angle is expressed in degrees and is measured counterclockwise from the positive x-direction.
- **Contours:** The **Data Editor** displays contours based on the cell data. The **Contours** tab allows you to control the display of the contour levels, labels and colors. The options of this tab are listed below.
  - **Visible:** Contours are visible if this box is checked.
  - **Display contour lines**: Contour lines (and labels) are displayed if this box is checked.
  - **Fill contours:** Checking this box causes the space between contour lines to be filled with the color defined in the contour level table.

- **Orient label uphill**: If this box is checked, the contour labels are displayed so that they are always oriented uphill (i.e., oriented to places with higher cell values).

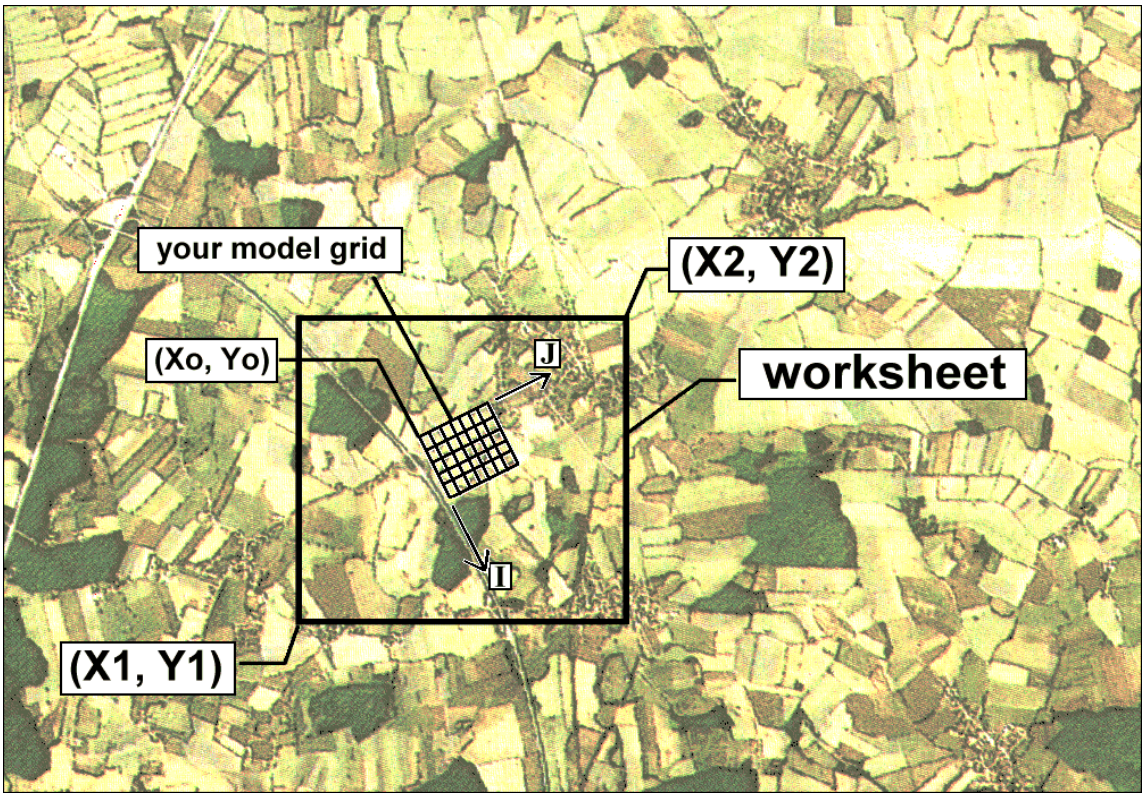


Fig. 3.63 Defining the location and orientation of the worksheet and model grid

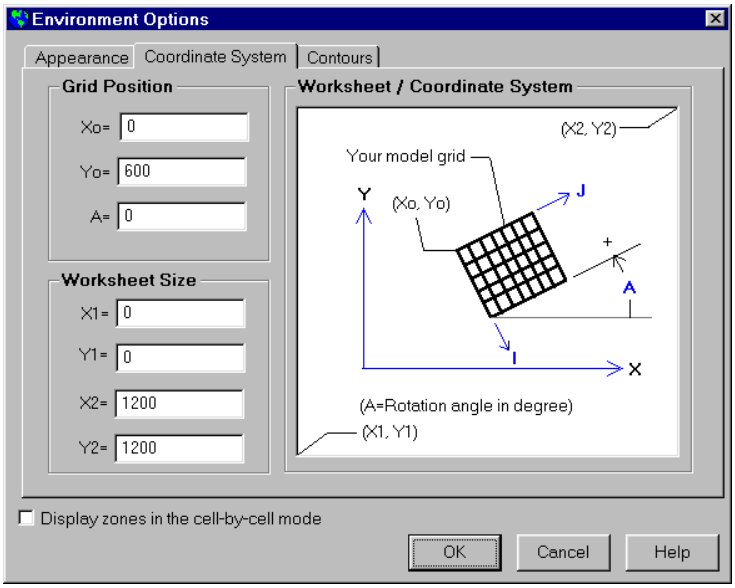


Fig. 3.64 The **Coordinate System** tab of the **Environment Options** dialog box

- **Ignore inactive cells**: If this box is checked, the data of inactive cells will not be used for creating contours.
- **Parameter:** If you are editing a particular package, in which a cell has more than one value (for example, the River package requires three values for each cell), you can select the parameter type from this drawdown box. PMWIN uses the data associated with the selected parameter type to create contours.
- **Contour level table:** You can click on each cell of the table and modify the values or you can click on the header button of each column of the table to change the values for all cells of the column.
  - **Level**: To produce contours on regular intervals, click the header of this column. A **Contour Levels** dialog box allows you to specify the contour range and interval. By default, this dialog box displays the maximum and minimum values found in the current layer. After having made your changes and clicked on **OK**, the contour levels in the table are updated to reflect the changes.
  - **Line** and **Fill** define the color of a contour line and the fill color between two contour lines. Clicking on one of the headers, the **Color Spectrum** dialog box (Fig. 3.66) appears. Using this dialog box, the contour colors can be automatically assigned to produce a gradational change from a minimum color to a maximum color. To change the minimum or maximum color, simply click on the button and select a color from a **Color** dialog box. After clicking on **OK**, a gradation of colors from the minimum to the maximum is assigned to each contour level.
  - **Label:** Using the **Contour Labels** dialog box (Fig. 3.67), you can define the display frequency of contour labels. **First labeled contour line** defines the first contour line to be labeled. **Labeled line frequency** specifies how often the contour lines are labeled. After having made your changes and clicked on OK, the flags in the table is updated to reflect the changes you specified. You can click on an individual cell of the label column to turn label on ☒ or off ☐.
  - **Label height** specifies the appearance height of the label text. It uses the same length unit as the model.
  - **Label spacing** specifies the distance between two contour labels. It uses the same length unit as the model.
- **Label Format**: The **Label Format** dialog box (Fig. 3.68) allows you to specify the format for the labels.
  - The **Fixed** option displays numbers at least one digit to the left and N digits to the right of the decimal separator, where N is the value specified in **Decimal digits**.

- The **Exponential** option displays numbers in scientific format and E is inserted between the number and its exponent.
- **Decimal digits** determines the number of digits to the right of the decimal separator. For example, if **Decimal digits** = 2, the value 1241.2 will be displayed as 1241.20 for the **fixed** option or 1.24E+03 for the **exponential** option.
- **Prefix** is a text string that appears before each label.
- **Suffix** is a text string that appears after each label.

- **Restore Defaults**: Clicking on this button, PMWIN sets the number of contour lines to 11 and uses the maxmum and minimum values found in the current layer as the minimum and maximum contour levels. The label height and spacing will also be set to their default values.
- **Load** and **Save**: The contents of the contour level table can be loaded from or saved in separate Contour files. Refer to Appendix 2 for the format.

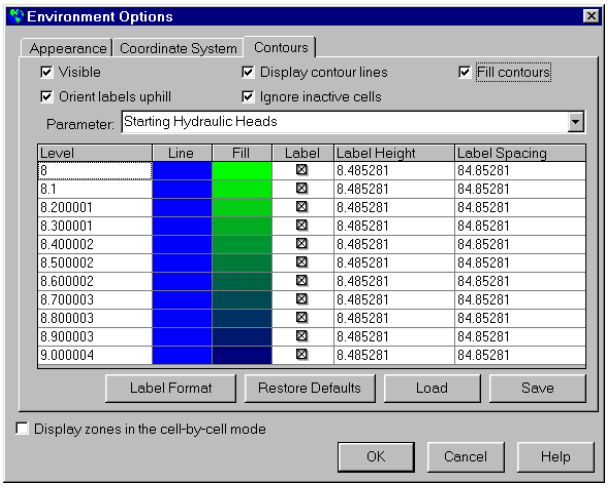


Fig. 3.65 The **Contours** tab of the **Environment Options** dialog box

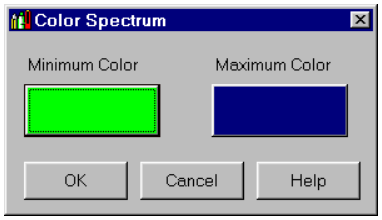


Fig. 3.66 The **Color Spectrum** dialog box

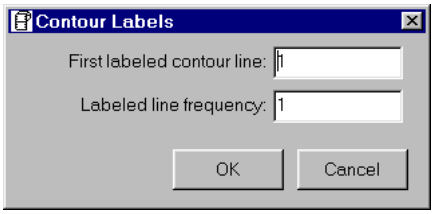


Fig. 3.67 The **Contour Labels** dialog box

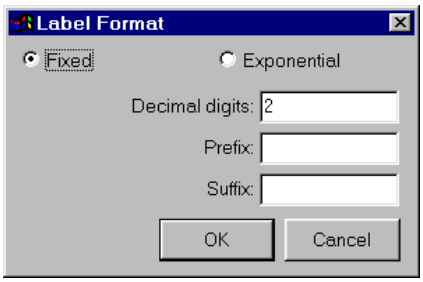


Fig. 3.68 The **Label Format** dialog box

Maps...

The **Maps Options** dialog box (Fig. 3.69) allows you to display up to 5 background DXF-maps, 3 Line maps and one geo-referenced raster (bitmap) graphics. The options in this dialog box are grouped under two tabs described below.

- **Vector Graphics**

  A **DXF-file** contains detailed data describing numerous CAD entities. An entity is a line or symbol placed on a drawing by the CAD system. PMWIN supports the following entities: LINE, POLYLINE, POINT, ARC, SOLID, CIRCLE and TEXT. The other entities will be ignored. There is no size limit to the number of the acceptable entities.

  A **Line Map** consists of a series of polylines. Each polyline is defined by a header line and a series of coordinate pairs. The header line only contains the number of the coordinate pairs. Refer to Appendix 2 for the format of the Line Map files.

  - **To import a DXF-map or a Line map:**

1. Select the **Vector Graphics** tab.
2. Click the *right* mouse button on any of the **DXF File** or **Line Map File** edit fields and select a file from a **Map Files** dialog box.

3. If necessary, use a scale factor to enlarge or reduce the appearance size of the map. Then use the values in X and Y to shift the **scaled** map to the desired position. For details, see **Scaling a vector graphic** below.
4. Click the colored button in the front of the edit field and select a color for the DXF-map from a **Color** dialog box. The color will be assigned to a DXF-graphics entity, if the entity's color is not defined in the DXF file. A line map will always use the selected color.
5. Check the check box next to the edit field. The map will be displayed only when the box is checked.

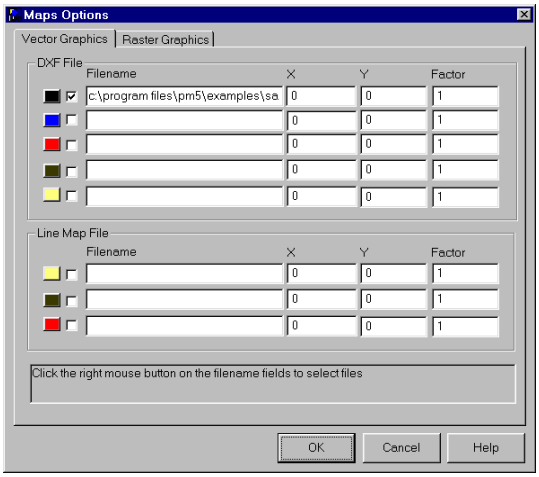


Fig. 3.69 The **Maps Options** dialog box

▸ **Scaling a vector graphic**

X and Y should be 0 and Scale should be 1, if a DXF file is generated by PMWIN or PMPATH. Because of different length units, DXF files created by some drawing or CAD software may not be imported into PMWIN without modifying the scale factor and the X, Y values. If these values are incorrect, a DXF-map will be displayed too small, too large or outside the worksheet. If this happens, use the **Environment options** dialog box to define a very large worksheet ensuring that the map can be displayed within the worksheet. Then, you can check the units on the imported map by moving the mouse around the map and looking at the X and Y coordinates displayed in the status bar. Choose two points that are a known distance apart and check their distance with the status bar. If the distance is incorrect, compute a scale factor and import the map again. Once you have the correct scale factor, you may shift the **scaled** DXF-map to the desired position by using X and Y. Fig. 3.70 uses a triangle as an example to show the use of X, Y and the scale factor.

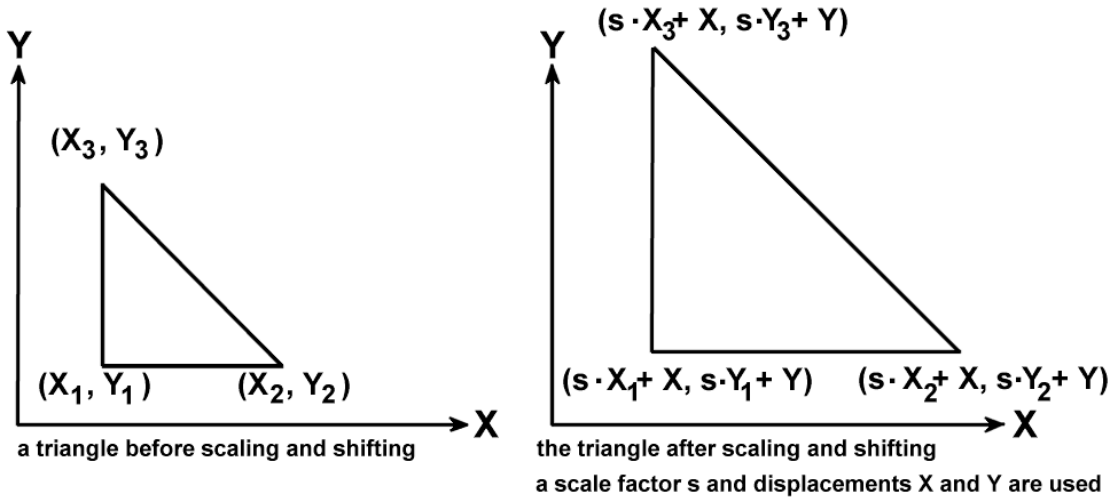


Fig. 3.70 Scaling a vector graphic

- **Raster Graphics**

  Raster graphics saved in Windows Bitmap (*.bmp) or JPEG (*.jpg) format can be imported and geo-referenced.

  - **To import a raster graphic**

1. Click the **Raster Graphics** tab.
2. Click the open file button and select a file from a **Raster Graphics** dialog box.
   The map is displayed in the **Maps Options** dialog box (Fig. 3.71). You can increase or decrease the magnification level of the display.
   - To **zoom in**, hold down the Shift-key and click the image with the left mouse button.
   - To **zoom out**, hold down the Ctrl-key and click the image with the right mouse button.
   - To **display entire map**, hold down the Alt-key and left-click the image.
   - To move a part of the image to the center of the display, simply left-click the desired position.

  - **To set geo-reference points**

1. Click the **Set** button from the **Point 1** or **Point 2** group.
   The mouse cursor turns into a crosshairs.
2. Place the crosshairs at a point with known (x, y) real-world coordinates and press the left mouse button.
3. Enter the (x, y) coordinates into the corresponding edit fields of the group **Point 1** or **Point 2**.

4. Repeat the steps 1 to 3 to set the other reference point. Note that the geo-reference points must not lie on a vertical or horizontal line, e.g., the x- and y-coordinates of the points must not be the same.

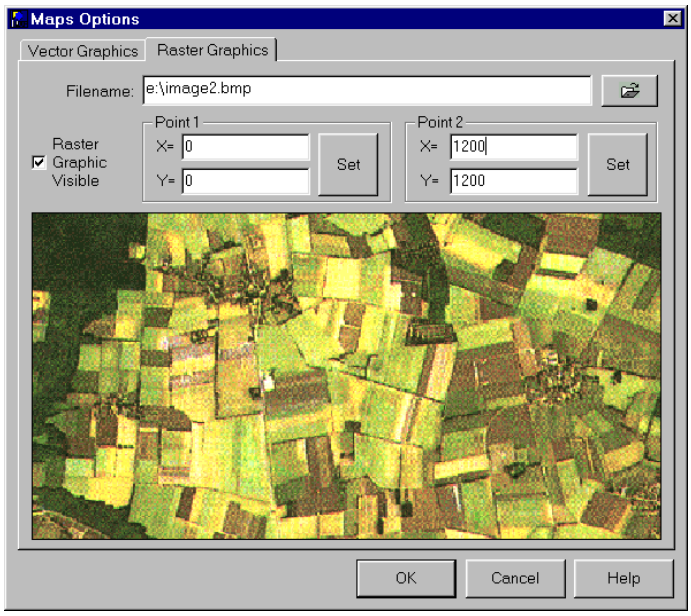


Fig. 3.71 Importing a geo-referenced raster map

FOR YOUR NOTES

4. The Advective Transport Model PMPATH

PMPATH is an advective transport model running independently from PMWIN. PMPATH retrieves the groundwater models and simulation result from PMWIN and MODFLOW. A semi-analytical particle tracking scheme (Pollock, 1988, 1989) is used to calculate the groundwater paths and travel times. Through the interactive graphical modeling environment of PMPATH, you can place particles and perform particle tracking with just a few mouse clicks. While most available particle tracking models need postprocessors for visualization of computed paths and times data, PMPATH calculates and animates the pathlines simultaneously (Fig. 4.1). Moreover, PMPATH provides various on-screen graphical options including head contours, drawdown contours and velocity vectors for any selected model layer and time step.

Both forward and backward particle tracking are allowed for steady-state and transient flow simulations. For transient flow simulations, particles can start from the beginning of any time step. During the simulation, the particle tracking algorithm will check the current time of every particle. If a particle reaches the end (forward tracking) or the beginning (backward tracking) of a time step, PMPATH forces the particle to wait, until the flow field of the next time step has been read. The particle tracking simulation proceeds until all particles have left the model via sinks or until the user-specified time limit is reached.

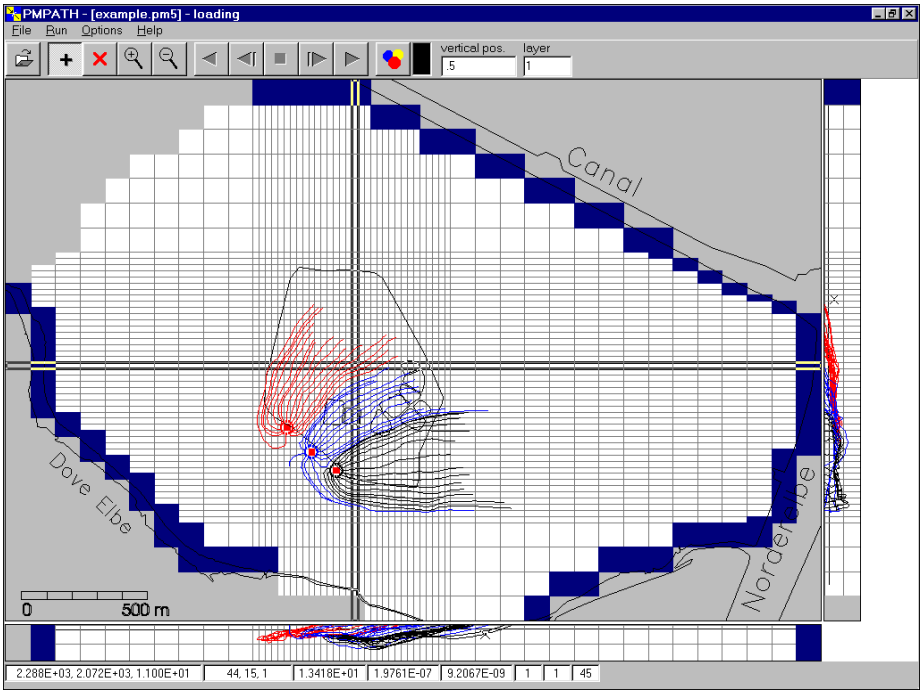


Fig. 4.1 PMPATH in operation

The time length of a single particle tracking step and the maximum number of tracking steps can be specified. Each particle can have its own color and retardation factor. With these features, PMPATH can be used to simulate advective transport in groundwater, to delineate contaminant capture zones, injection zones and wellhead protection areas or to find the point of origin of water in specified zones. PMPATH creates several output files including hydraulic heads distribution, velocity field, the x,y,z coordinates and travel times of particles. Graphics output includes DXF, HPGL and BMP (Windows bitmap) formats. Due to PMPATH's intensive graphical capability, there is no need for additional packages for graphical representations of the simulation results.

4.1 The Semi-analytical Particle Tracking Method

Assume that the density of groundwater is constant. Consider a unit volume of a porous medium as shown in Fig. 4.2 and apply Darcy's law and the law of conservation of mass. The three dimensional form of the partial differential equation for transient groundwater flow in saturated porous media can be expressed as

$$\frac{\partial v_{sx}}{\partial x} + \frac{\partial v_{sy}}{\partial y} + \frac{\partial v_{sz}}{\partial z} - w = S_s \frac{\partial h}{\partial t} \qquad (4.1)$$

where

v_{sx}, v_{sy} and v_{sz} [L/T] are values of the specific discharge (or Darcy velocity) through the unit volume along the x, y, and z coordinate axes;

w [1/T] is a volumetric flux per unit volume and represents internal sources and/or sinks of water;

S_s [1/L] is the specific storage of saturated porous media;

h [L] is the hydraulic head; and

t [T] is time.

For a three-dimensional finite-difference cell as shown in Fig. 4.3, the finite-difference form of eq. 4.1 can be written as

$$\frac{(Q_{x2} - Q_{x1})}{(\Delta y \cdot \Delta z) \cdot \Delta x} + \frac{(Q_{y2} - Q_{y1})}{(\Delta x \cdot \Delta z) \cdot \Delta y} + \frac{(Q_{z2} - Q_{z1})}{(\Delta x \cdot \Delta y) \cdot \Delta z} = \frac{W}{\Delta x \cdot \Delta y \cdot \Delta z} + S_s \frac{\Delta h}{\Delta t} \qquad (4.2)$$

where

Q_{x1}, Q_{x2}, Q_{y1}, Q_{y2}, Q_{z1} and Q_{z2} [L^3T^{-1}] are volume flow rates across the six cell faces.
Δx, Δy and Δz [L] are the dimensions of the cell in the respective coordinate directions;
W [L^3T^{-1}] is flow to internal sources or sinks within the cell; and
Δh [L] is the change in hydraulic head over a time interval of length Δt [T].

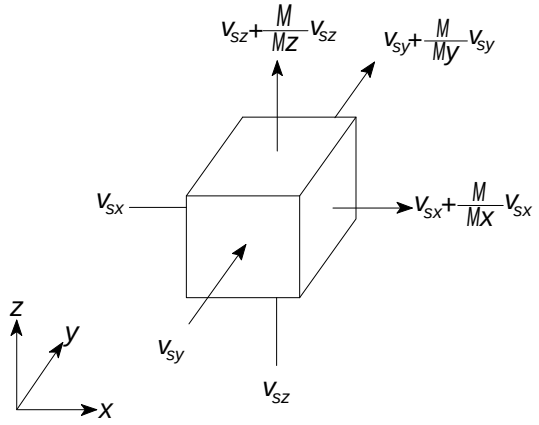


Fig. 4.2: Flow through a unit volume of a porous medium

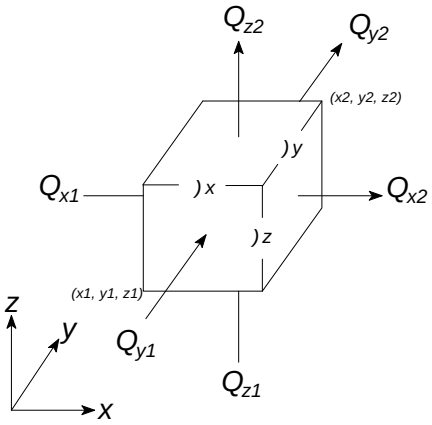


Fig. 4.3: Finite-difference approach

Eq. 4.2 is the mass balance equation for a finite-difference cell. The left hand side of eq. 4.2 represents the net mass rate of outflow per unit volume of the porous medium, and the right hand side is the mass rate production per unit volume due to internal sources/sinks and mass storage. Substitution of Darcy's law for each flow term in eq. 4.2, ie, $Q=\Delta h \cdot K \cdot A/\Delta x$, yields an equation expressed in terms of (unknown) heads at the center of the cell itself and adjacent cells. An equation of this form is written for every cell in the mesh in which head is free to vary with time. Once the system of equations is solved and the heads are obtained, the volume flow rates across the cell faces can be computed from Darcy's law. The average pore velocity components across each cell face are

$$v_{x1} = Q_{x1} / (n \cdot \Delta y \cdot \Delta z) \quad (4.3a)$$
$$v_{x2} = Q_{x2} / (n \cdot \Delta y \cdot \Delta z) \quad (4.3b)$$
$$v_{y1} = Q_{y1} / (n \cdot \Delta x \cdot \Delta z) \quad (4.3c)$$
$$v_{y2} = Q_{y2} / (n \cdot \Delta x \cdot \Delta z) \quad (4.3d)$$
$$v_{z1} = Q_{z1} / (n \cdot \Delta x \cdot \Delta y) \quad (4.3e)$$
$$v_{z2} = Q_{z2} / (n \cdot \Delta x \cdot \Delta y) \quad (4.3f)$$

where

n [-] is the effective porosity, and

v_{x1}, v_{x2}, v_{y1}, v_{y2}, v_{z1}, and v_{z2} [LT^{-1}] are the average pore velocity components across each cell face.

Pollock's semi-analytical particle tracking scheme is based on the assumption that each directional velocity component varies linearly within a model cell in its own coordinate direction. The semi-analytical particle tracking algorithm uses simple linear interpolation to compute the principle velocity components at any points within a cell. Given the starting location (x, y, z) of the particle and the starting time t_1, the velocity components are expressed in the form

$$v_x(t_1) = A_x(x - x_1) + v_{x1} \quad (4.4a)$$
$$v_y(t_1) = A_y(y - y_1) + v_{y1} \quad (4.4b)$$
$$v_z(t_1) = A_z(z - z_1) + v_{z1} \quad (4.4c)$$

where x_1, y_1 and z_1 are defined in Fig. 4.3. A_x, A_y and A_z [T^{-1}] are the components of the velocity gradient within the cell,

$$A_x = (v_{x2} - v_{x1}) / \Delta x \quad (4.5a)$$
$$A_y = (v_{y2} - v_{y1}) / \Delta y \quad (4.5b)$$
$$A_z = (v_{z2} - v_{z1}) / \Delta z \quad (4.5c)$$

Using a direct integration method described in Pollock (1988) and considering the movement of the particle within a cell, the particle location at time t_2 is

$$x(t_2) = x_1 + (v_x(t_1) \cdot e^{A_x \cdot \Delta T} - v_{x1}) / A_x \quad (4.6a)$$
$$y(t_2) = y_1 + (v_y(t_1) \cdot e^{A_y \cdot \Delta T} - v_{y1}) / A_y \quad (4.6b)$$
$$z(t_2) = z_1 + (v_z(t_1) \cdot e^{A_z \cdot \Delta T} - v_{z1}) / A_z \quad (4.6c)$$

where $\Delta T = t_2 - t_1$

For steady-state flow fields, the location of the particle at time t_2 must be still within the same cell as at time t_1. Given any particle's starting location within a cell at time t_1, Pollock's algorithm allows to determine the particle's exit time t_2 and exit point from the cell directly, without having to calculate the actual path of the particle within the cell.

The particle tracking sequence is repeated until the particle reaches a discharge point or until a user-specified time limit is reached. Backward particle tracking is implemented by multiplying

all velocity terms in equations 4.3a - 4.3f by -1.

For transient flow fields, in addition to the condition for steady-state flow fields, t_1 and t_2 must lie within the same time step. In PMPATH, each particle may be associated with a set of attributes, i.e., the retardation factor, the starting, forward and backward travel times and positions. If a particle is travelling across the end (forward tracking) or the beginning (backward tracking) of a time step of a flow simulation, PMPATH sets t_2 to the end or beginning time of this time step and forces the particle to wait until the flow field of the next time step (forward tracking) or the previous time step (backward tracking) is read. If the end or beginning time of a transient flow simulation is reached, the most recent flow field can be treated as steady-state and the movement of particles can go on.

Consideration of the display of the calculated pathlines

Because of the capability of calculating particle's exit point from a cell directly, pathlines displayed by PMPATH may sometimes intersect each other. Consider the case shown in Fig. 4.4, two particles within a two-dimensional cell start at the same time. The dashed curves represent the actual paths of these two particles. The solid lines are the pathlines displayed by PMPATH. The pathlines intersect each other, although the particles' exit points are exactly equal to that of the actual paths. This effect can be prevented by using a smaller particle tracking step length such that intermediate particle positions between starting point and exit point can be calculated. See **Particle Tracking (Time) Properties** dialog box (sec. 4.3) for how to change the particle tracking step length.

Consideration of the spatial discretization and water table layers

The method described above is based on the assumption that the model domain was discretized into an orthogonal finite-difference mesh, i.e., all model cells in the same layer have the same thickness. In practice, variable layer thickness is often preferred for approaching varying thicknesses of stratigraphic geohydrologic units. In order to calculate approximate groundwater paths for this kind of discretization, PMPATH (as well as MODPATH) uses a vertical local coordinate instead of the real-world z-coordinate. The vertical local coordinate is defined for each cell as

$$z_L = (z - z_1) / (z_2 - z_1) \tag{4.7}$$

where z_1 and z_2 are the elevations of the bottom and top of the cell, respectively. According to this equation, the vertical local coordinate z_L is equal to 0 at the bottom of the cell and z_L is equal

to 1 at the top of the cell. When a particle is moved laterally from one cell to another, its vertical local coordinate remains unchanged, regardless of how the elevations of the bottom and top vary from one cell to another.

In MODFLOW, model layers of type 1 (unconfined) are always water table layers, model layers of type 2 or 3 (confined/unconfined) are water table layers when the head in the cell is beneath the elevation of the cell top. For water table layers, z_2 is set equal to the head in the cell.

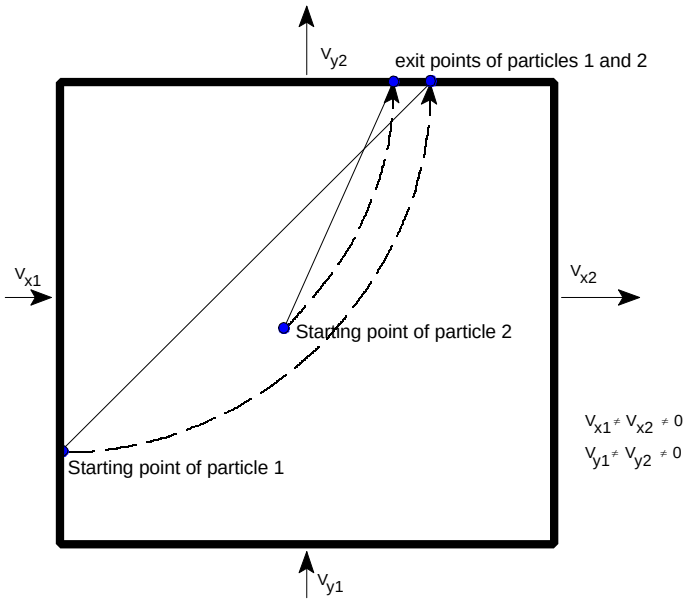


Fig. 4.4: Schematic illustration of the spurious intersection of two pathlines in a two-dimensional cell.

4.2 PMPATH Modeling Environment

The PMPATH modeling environment (Fig. 4.5) consists of the Worksheet, the cross-section windows, the tool bar and and the status bar. They are described below.

Worksheet and cross-section windows

PMPATH as well as PMWIN use the same spatial discretization convention as used by MODFLOW. An aquifer system is discretized into mesh blocks, or cells. An I, J, K indexing system is used to describe the locations of cells in terms of rows, columns and layers. The I-, J-, and K- axes are oriented along the row, column and layer direction, respectively. The origin of

the cell indexing system is located at the upper, top, left cell of the model. MODFLOW numbers the layers from the top down, an increment in the K index corresponds to a decrease in elevation z.

PMPATH always displays the model grid parallel to the Worksheet, while PMWIN allows a user to shift and rotate a model grid by giving the rotation angle A and the coordinates (x_0, y_0) of the upper-left corner of the grid. The relation between the model grid and the real-world (x, y, z) coordinate system is illustrated in Fig. 4.5. The Worksheet displays the plan view of the current model layer and the projection of pathlines on the horizontal IJ-plane. The cross-section windows display the projection of pathlines on the IK- and JK-planes. The **Environment Options** dialog box of PMPATH (see sec. 4.3) allows the user to change the appearance of these windows.

The projection of pathlines on the cross-sections is useful when running PMPATH with a three-dimensional (multi-layer) flow field. One should always keep in mind that only the *projections* of pathlines are displayed. The projection of a pathline may be intersected by another or even itself, particularly if a three-dimensional flow field or a transient flow field is used.

Status bar

The Statusbar displays the following messages:

1. the current position of the mouse cursor (in both [x, y, z] coordinates and [J, I, K] indices);
2. the hydraulic head at the cell [J, I, K];
3. the average horizontal pore velocity at the center of the cell [J, I, K];
4. the average vertical pore velocity at the center of the cell [J, I, K];
5. the current stress period of the flow simulation;
6. the current time step of the flow simulation; and
7. the number of particles.

See **Particle Tracking (Time) Properties** dialog box (sec. 4.3) for how to change the current stress period and time step. The hydraulic heads at the current stress period and time step are calculated by MODFLOW. The average horizontal pore velocity at the center of a cell is obtained by averaging the velocities v_{x1}, v_{x2} and v_{y1}, v_{y2} respectively (see equation 4.3a-4.3d). The average vertical pore velocity at the center of a cell is the average of the velocities v_{z1}, v_{z2} (see equation 4.3e and 4.3f). The vertical velocity is defined as positive when it points in the k-direction.

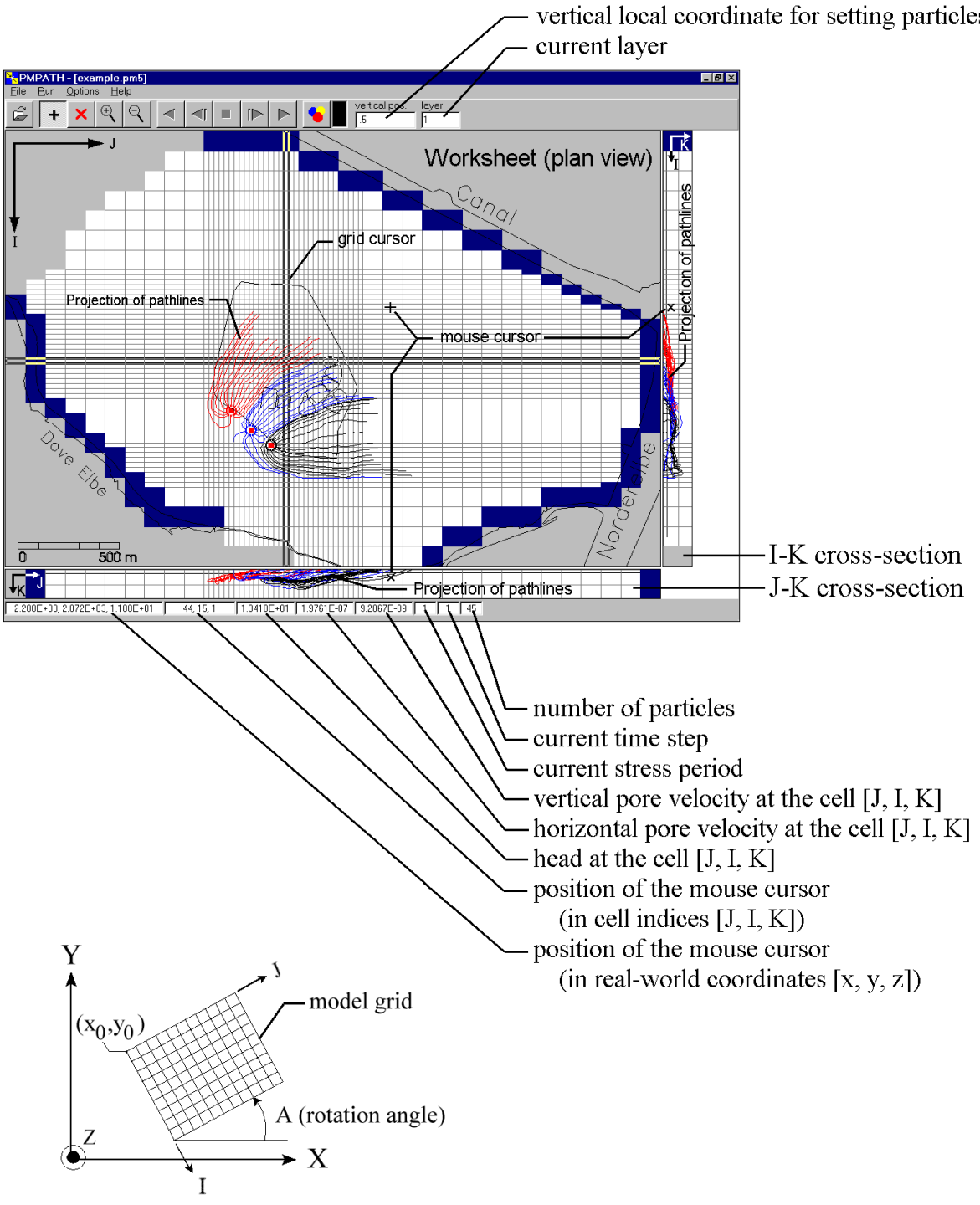


Fig. 4.5: The PMPATH modeling environment

Tool bar

The tool bar provides quick access to commonly used commands in the PMPATH modeling environment. You click a button on the tool bar once to carry out the action represented by that button. To change the current layer or the vertical local coordinate, click the corresponding edit field in the tool bar and type the new value then press ENTER. See eq. 4.7 for the definition of the vertical local coordinate. The following table summarizes the use of the tool bar buttons of PMPATH.

Table 4.1 Summary of the tool bar buttons of PMPATH

Button	Action
	**Open Model**; allows a user to open a model created by PMWIN.
	**Set Particle**; allows a user to place particles in the model domain.
	**Erase Particle**; provides a way to delete particles.
	**Zoom In**; allows you to drag a zoom-window over a part of the model.
	**Zoom Out**; Forces PMPATH to display the entire model grid.
	**Particle color**; Allows a user to select a color for new particles from a **color** dialog box.
	**Run particles backward**; executes backward particle tracking for a time lenght. The time length is defined by the product of the number of particle tracking steps and the particle tracking step length.
	**Run particles backward step by step**; executes backward particle tracking for a user-specified particle tracking step length.
	**Stop**; stops the particle tracking or stops drawing particles.
	**Run particles forward step by step**; executes backward particle tracking for a user-specified particle tracking step length.
	**Run particles forward**; executes forward particle tracking for a time length. The time length is defined by the product of the number of particle tracking steps and the particle tracking step length.

 Open model

Opens an existing model created by PMWIN. A PMWIN-model file always has the extension **PM5**. Prior to openning a model, the flow simulation must be performed. By default, PMPATH reads the unformatted (binary) files (HEADS.DAT and BUDGET.DAT) from the same folder as the loaded model.

 Set particle

Use the following two methods to place particles in the current layer. The current layer is shown in the tool bar (Fig. 4.5). Change it first, if you need to place particles into another layer. Note that particles cannot be placed in inactive cells or fixed-head cells (constant head cells).

- **To place a group of particles**

1. Click the **Set particle** button [+].
2 Move the mouse cursor to the active model area. The mouse cursor turns into crosshairs.
3. Place the crosshairs where you want a corner of the "Set Particle" window.
4. Drag the crosshairs until the window covers the subregion over which particles will be placed, then release the mouse button.

   The **Add New Particles** box appears (Fig. 4.6). Where NI, NJ and NK are the number of particles in I, J and K directions, respectively. Using NI, NJ and NK, particles can be placed either on cell faces or within cells which lie in the "Set Particle" window.These numbers can range from 0 to 999. In the case shown in Fig. 4.6, 8 particles will be placed within each cell, 3 (=3×1) particles will be placed on each cell face and 15 particles will be placed around each cell at a distance of 20. The particles will get the color and the retardation factor given in the Properties tab of this dialog box.

- **To place a single particle**

1. Click the **Set particle** button [+].
2. Change the vertical local coordinate and the particle color (for the definition of the vertical local coordinate, see equation 4.7).
3. Move the mouse cursor to the desired position and click the *right* mouse button. A particle will be placed. Note that this particle will have the retardation factor specified in the Properties tab of the **Add New Particles** dialog box. Once particles are placed, their color and retardation factor cannot be changed any more.

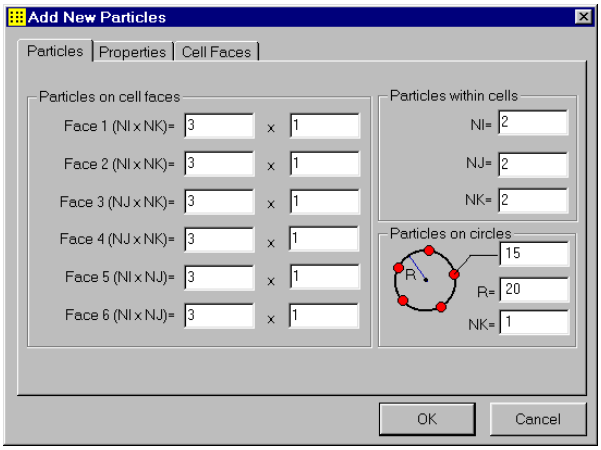


Fig. 4.6: The **Add New Particles** dialog box

The retardation factor R is defined by

$$R = 1 + \frac{\rho_b}{n} \cdot K_d \qquad (4.8)$$

where ρ_b is the bulk mass density of the porous medium, n is the effective porosity, and K_d is the distribution coefficient. A detailed description of these parameters can be found in the literature, e.g., Freeze and Cherry (1979). The retardation factor was first applied to groundwater problems by Higgins (1959) and Baetsle (1967). Baetsle indicated that it may be used to determine the retardation of the center of mass of a contaminant moving from a point source while undergoing adsorption. PMPATH uses the retardation factor to modify the average pore velocity of the groundwater flow. The velocity vectors in equation (4.3a)-(4.3f) become

$$v_{x1} = Q_{x1} / (n \cdot \Delta y \cdot \Delta z) / R \qquad (4.9a)$$
$$v_{x2} = Q_{x2} / (n \cdot \Delta y \cdot \Delta z) / R \qquad (4.9b)$$
$$v_{y1} = Q_{y1} / (n \cdot \Delta x \cdot \Delta z) / R \qquad (4.9c)$$
$$v_{y2} = Q_{y2} / (n \cdot \Delta x \cdot \Delta z) / R \qquad (4.9d)$$
$$v_{z1} = Q_{z1} / (n \cdot \Delta x \cdot \Delta y) / R \qquad (4.9e)$$
$$v_{z2} = Q_{z2} / (n \cdot \Delta x \cdot \Delta y) / R \qquad (4.9f)$$

Erase particle

You can only erase particles located in the current layer. The current layer is shown in the tool bar. Change it first, if you need to erase particles in another layer.

▸ **To delete particles**

1. Click the **Erase particle** button .
2. Move the mouse cursor to where you want a corner of the "Erase" window.
3 Drag the mouse cursor until the window covers the particles which will be deleted.
4. Release the mouse button.

Zoom In

By default, PMPATH displays the entire model grid. **Zoom in** is useful, if you want to view a part of the model domain in greater detail or if you want to save plots of a certain part of the model area (see Sec 4.4 for how to save plots).

▸ **To zoom in on a part of the model**

1. Click the **Zoom In** button  .
2. Move the mouse cursor to where you want a corner of the "Zoom" window.
3 Drag the mouse cursor until the window covers the model area which is to be displayed.
4. Release the mouse button.

 **Zoom Out**

Clicking on the "Zoom out" button forces PMPATH to display the entire model grid.

 **Particle color**

Clicking on the **Particle color** button allows a user to select a color for new particles from a **Color** dialog box. Particles with different colors are useful when, for example, you want to determine the capture zones of several pumping wells. In this case, particles with a certain color are placed around or on the cell-faces of each pumping well. Through backward tracking, capture zones of each pumping well can be recognized by their different colors.

 **Run particles backward**

Click this button to execute backward particle tracking for a specified time length. The time length is the product of the number of particle tracking steps and the particle tracking step length given in the **Particle Tracking (Time) Properties** dialog box. See sec. 4.3 for details.

 **Run particles backward step by step**

Click this button to move particles backward a single particle tracking step. The particle tracking step length is defined in the **Particle Tracking (Time) Properties** dialog box. See sec. 4.3 for details.

 **Stop**

You can click the **Stop** button to stop particle tracking or stop redrawing particles when the **Stop** button is highlighted (ie, the rectangle on the button is colored in red).

PMPATH redraws the particles whenever the PMPATH window has been covered by other windows and becomes visible again. For example, if you change to another application and then return to PMPATH, PMPATH will redraw all particles. If too many particles are placed, you will need to keep PMPATH from redrawing all particles. Under some circumstances, PMPATH will take a long time for calculating the coordinates of flow paths and travel times. This is especially true, if the flow velocities and the user-specified time step length of particle tracking are very

small. Click the **Stop** button, if the particle tracking simulation appears too slow.

Run particles forward step by step

Click this button to move particles forward a single particle tracking step. The particle tracking step length is defined in the **Particle Tracking (Time) Properties** dialog box. See sec. 4.3 for details.

Run particles forward

Click this button to execute forward particle tracking for a specified time length. The time length is the product of the number of particle tracking steps and the particle tracking step length given in the **Particle Tracking (Time) Properties** dialog box. See sec. 4.3 for details.

4.3 PMPATH Options Menu

Environment...

The **Environment Options** dialog box (Fig. 4.7) allows to modify the appearance of the model. The available settings are grouped under 4 tabs; namely Appearance, Cross Sections, Velocity vectors and Contours. These tabs are described below.

- **Appearance** allows to change the visibility and appearance color of each simulated component. A simulated component is visible if the corresponding **Visibility** check box is checked. To select a new color, click on the colored cell (a button appears), then click on the button and select a color from a **Color** dialog box.
- **Cross Sections**
  - To display the cross-section windows, check the **Visible** check box.
  - To display the model grid, check the **Show grid** check box.
  - To display the groundwater surface (or the hydraulic heads of the highest active cells) on the cross-sections, check the **Groundwater surface (Potential)** check box.
  - Use **Exaggeration** (scaling factor for the height) to change the appearance height of the cross-sections. A larger exaggeration value lets you see the projection of the pathlines on the cross-section windows in greater details. The exaggeration value can be ranged from 0.01 to 1000. If the model thickness or the exaggeration value is too small such that the appearance size on the screen is smaller than 1 pixel, PMPATH will turn off the display

of the cross sections. In this case, the **Visible** check box will be unchecked automatically.

- **Projection Row** and **Projection Column**: PMPATH uses a *grid cursor* to define the column and row for which the cross-sectional plots should be made. You can move the grid cursor by holding down the Ctrl-key and click the left mouse button on the desired position. Alternatively, you can type the row and column in the **Projection Row** and **Projection Column** edit boxes. The visible part on the cross-sectional plots is defined by **Minimum Elevation** and **Maximum Elevation**. By default, the maximum elevation is set to the highest elevation of the model grid (or the largest hydraulic head). The minimum elevation is set to the lowest elevation of the model grid (or the smallest hydraulic head).

▸ **Velocity vectors**

Velocity vectors describe the directions of water movement at any instant of a given time step of the simulation (The time step is defined by **Current Time** of the **Particle Tracking (Time) Properties** dialog box; see Fig. 4.11). Check the **Visible** check box, the projection of velocity vectors of each active model cell will be displayed on the Worksheet and cross-section windows. Click the color button next to the **Visible** check box to change the appearance color of the velocity vectors. The appearance size of the largest velocity vector is defined by the **Vector size** (in pixels), which defaults to 25 and can be ranged from 1 to 32767.

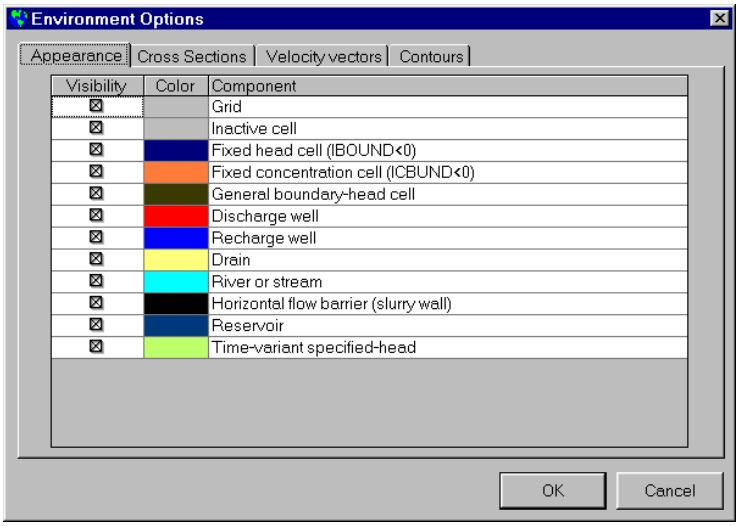


Fig. 4.7 The **Environment Options** dialog box

- **Contours:**

  PMPATH displays contours based on the calculated heads or drawdowns. The **Contours** tab allows you to control the display of the contour levels, labels and colors. The options of this tab are listed below.

  - **Visible:** Contours are visible if this box is checked.
  - **Orient label uphill**: If this box is checked, the contours labels are displayed so that they are always oriented uphill (i.e., oriented to places with higher cell values).
  - **Head** or **Drawdown**: Use the options **Head** or **Drawdown** to decide which kind of contours should be displayed.
  - **Contour level table:** You can click on each cell of the table and modify the values or you can click on the header button of each column of the table to change the values for all cells of the column.
    - **Level**: To produce contours on regular intervals, click the header of this column. A **Contour Levels** dialog box allows you to specify the contour range and interval. By default, this dialog box displays the maximum and minimum values found in the current layer. After having made your changes and clicked on **OK**, the contour levels in the table are updated to reflect the changes.
    - **Color** defines the color of a contour line. Clicking on the header, the **Color Spectrum** dialog box (Fig. 4.8) appears. Using this dialog box, the contour colors can be automatically assigned so you get a gradational change from a minimum color to a maximum color. To change the minimum or maximum color, simply click on the button and select a color from a **Color** dialog box. After clicking on **OK**, a gradation of colors from the minimum to the maximum is assigned to each contour level.
    - **Label:** Using the **Contour Labels** dialog box (Fig. 4.9), you can define the display frequency of contour labels. **First labeled contour line** defines the first contour line to be labeled. **Labeled line frequency** specifies how often of the contour lines are labeled. After having made your changes and clicked on OK, the flags in the table is updated to reflect the changes you specified. You can click on individual cell of the label column to turn label on ☒ or off ☐.
    - **Label height** specifies the appearance height of the label text. It uses the same length unit as the model.
    - **Label spacing** specifies the distance between two contour labels. It uses the same length unit as the model.
  - **Label Format**: The **Label Format** dialog box (Fig. 4.10) allows you to specify the format for the labels.
    - The **Fixed** option displays numbers at least one digit to the left and N digits to the

right of the decimal separator, where N is the value specified in **Decimal digits**.

- The **Exponential** option displays numbers in scientific format and E is inserted between the number and its exponent.
- **Decimal digits** determines the number of digits to the right of the decimal separator. For example, if **Decimal digits** = 2, the value 1241.2 will be displayed as 1241.20 for the **fixed** option or 1.24E+03 for the **exponential** option.
- **Prefix** is a text string that appears before each label.
- **Suffix** is a text string that appears after each label.

- **Restore Defaults**: Clicking on this button, PMPATH sets the number of contour lines to 11 and uses the maxmum and minimum values found in the current layer as the minimum and maximum contour levels. The label height and spacing will also be set to their default values.
- **Load** and **Save**: The contents of the contour level table can be load from or save in separate Contour files. Refer to Appendix 2 for the format.

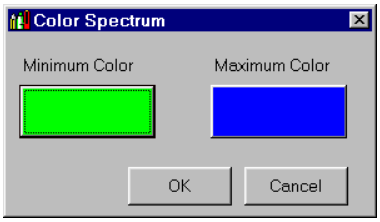


Fig. 4.8 The **Color Spectrum** dialog box

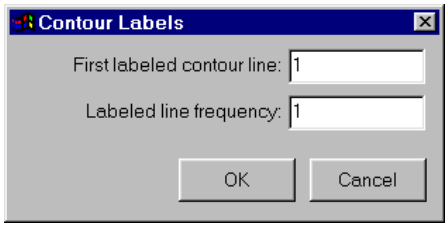


Fig. 4.9 The **Contour Labels** dialog box

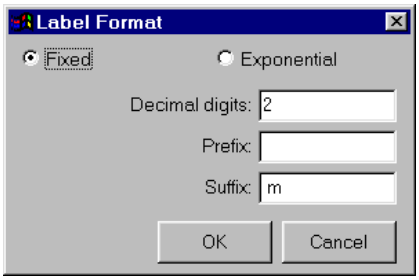


Fig. 4.10 The **Label Format** dialog box

Particle Tracking (Time)...

The available settings of the **Particle Tracking (Time)** dialog box (Fig. 4.11) are grouped under 3 tabs; namely Simulation Mode/Time, Pathline Colors and RCH/EVT options. These tabs are described below.

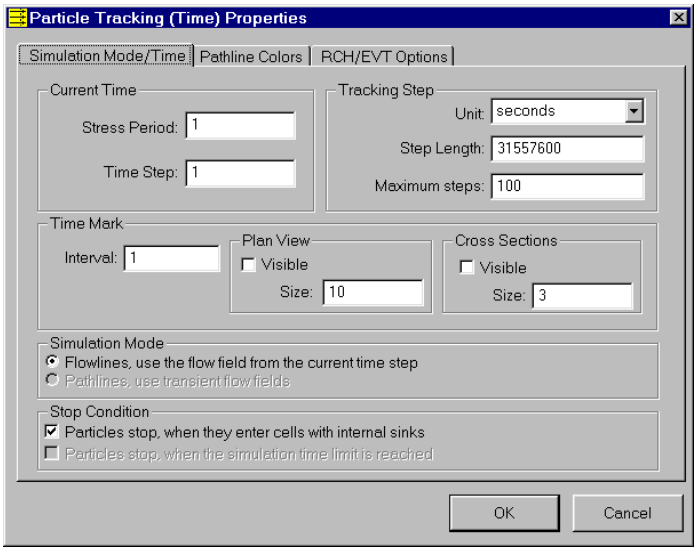


Fig. 4.11 The **Particle Tracking (Time) Properties** dialog box

- **Simulation Mode/Time**
  - **Current Time:** In MODFLOW, simulation time is divided into stress periods, which are in turn divided into time steps. The time length of each stress period and time step is defined in PMWIN. In PMPATH, you can move to any stress period and time step as long as the resulting heads and budget data are saved for that stress period/time step. The starting time of each particle is always the beginning of the time step defined in Current Time.
  - **Tracking Step:** To select a time unit for Step length, click the down arrow on the Unit drop-down box. The **step length** is the time length that particles may move when one of the buttons or is pressed. **Maximum steps** is the allowed number of particle tracking steps. Each time you press one of the buttons or , particles may move backward or forward for a time length defined by the product of **Step length** and **Maximum steps**.
  - **Time Mark**: PMPATH places a time mark on pathlines for each n-tracking step, where n is given in **Interval**. Check the corresponding **Visible** check boxes, if you want to see time marks on the Worksheet (plan view) or the cross-section windows. The appearance

size of the time marks is defined by **Size** (in pixels). The default value of Size is 10 for the top view window and 3 for the cross-section windows. The sizes can be ranged from 1 to 2,147,483,647.

- **Simulation Mode:** PMPATH can be used to calculate flowlines or pathlines. Flowlines indicate the instantaneous direction of flow throughout a system (at all times of a steady-state flow simulation or at a given time step of a transient flow simulation). Pathlines map the route that an individual particle of water follows through a region of flow during a steady-state or transient condition. In a steady-state flow system pathlines will coincide with flowlines. In this case, only the option **Flowline, use the flow field from the current time step** is available. In the case of a transient flow simulation that groundwater flow varies from time step to time step, the flowlines and pathlines do not coincide. Use the option **Pathlines, use transient flow fields** to calculate transient pathlines.
- **Stop Conditions:** In general, particles will stop when the allowed travel time defined in **Tracking Step** is reached or when the particles reach specified head cells. In addition to these conditions, two stop conditions are available:
  1. **Particles stop, when they enter cells with internal sinks:**
     The flow model MODFLOW includes the options to simulate wells, drains, rivers, general-head boundaries, streams, evapotranspiration and recharge. Except the last two options, they are treated as internal distributed sources or sinks by PMPATH. If the internal sink of a cell is sufficiently strong, flow will be into the cell from all cell faces. In that case, every particle that enters the cell will be discharged. If the sink is weak, flow will be into the cell from some cell faces and a part of flow will leave the cell through another faces. A particle entering such a cell may be discharged or may leave the cell again. In the finite-difference approach, however, it is impossible to determine whether that particle should be discharged or pass through the cell. If this option is selected, particles will be discharged when they enter cells with internal sinks, regardless of the flow condition.
  2. **Particles stop, when the simulation time limit is reached.**
     This option is only available, if the simulation mode **Pathlines, use transient flow fields** is selected. In PMPATH, the starting time of each particle is always the beginning of the time step defined in **Current Time**. For the forward particle tracking scheme, the simulation time limit is the end of a transient flow simulation. For the backward particle tracking scheme, on the other hand, the simulation time limit is the beginning of the simulation. Backward particle tracking will not work, if this stop option is checked and particles are started from the beginning of a transient flow

simulation. In this case, particles will be stopped immediately after the start. Note that you cannot start backward particle tracking from the end of a transient flow simulation, rather you can only start particles from the beginning of the last simulation time step. If the simulation time limit is reached and this option is not checked, PMPATH calculates flowlines by assuming that the flow field of the first or last time step is steady-state.

- **Pathline Colors:**

Normally, the color of each pathline is the same as the color of each particle. It is sometimes useful when the colors of pathlines are distinguished by layers instead of particles. There are two ways to change the color of each layer:

1. **Change the color individually**
   a. Click on a colored cell of the table, a button will appear in the cell.
   b. Click on the button then select a color from a **Color** dialog box.
2. **Change the color using the Color Spectrum** dialog box
   Using the **Color Spectrum** dialog box, the color of each layer can be automatically assigned so you get a gradational change from one color to another.
   a. Click the header button **Color**. A **Color Spectrum** dialog box appears.
   b. In the **Color Spectrum** dialog box, click the Minimum Color button to display a Color dialog box. In the Color dialog box, select a color and click OK. Repeat this procedure for the Maximum Color button.
   c. In the **Color Spectrum** dialog box, click OK. A gradation of colors from the minimum to the maximum is assigned to each layer.

- **RCH/EVT Options:**

- **Recharge**: The option is disabled if recharge is not used. MODFLOW treats recharge as an internal distributed source of a cell and does not assign it to any of the six cell faces. The distributed source approximation is usually only appropriate for two-dimensional areal flow models. The flow velocity across the top face of a cell in the top model layer would be zero, if the existing recharge is not assigned to the top face. Consequently, particles cannot be tracked backwards to the top face.

  In PMPATH, recharge may be treated as a distributed source, or assigned to the top face or bottom face of a cell by selecting a corresponding option from the dialog box. Recharge will be assigned to the top face and "negative" recharge will be assigned to the bottom face, if the option Assign recharge to top and bottom cell faces is chosen.
- **Evapotranspiration:** The option is disabled if evapotranspiration is not used. Similar to Recharge, evapotranspiration can be assigned to top face of a cell or treated as a distributed sink.

Maps...

The **Maps Options** dialog box (Fig. 4.12) allows to display up to 5 background DXF-maps and 3 Line maps. A **DXF-file** contains detailed data describing numerous CAD entities. An entity is a line or symbol placed on a drawing by the CAD system. PMWIN supports the following entities: LINE, POLYLINE, POINT, ARC, SOLID, CIRCLE and TEXT. The other entities will be ignored. There is no size limit to the number of the acceptable entities.

A **Line Map** consists of a series of polylines. Each polyline is defined by a header line and a series of coordinate pairs. The header line only contains the number of the coordinate pairs. Refer to Appendix 2 for the format of the Line Map files.

- **To import a DXF-map or a Line map:**

1. Click the *right* mouse button on any of the **DXF File** or **Line Map File** edit fields and select a file from a **Map Files** dialog box.
2. If necessary, use a scale factor to enlarge or reduce the appearance size of the map. Then use the values in X and Y to shift the **scaled** map to the desired position. For details, see **Scaling a vector graphic** in sec. 3.9.
3. Click the colored button in the front of the edit field and select a color for the DXF-map from a **Color** dialog box. The color will be assigned to a DXF-graphics entity, if the entity's color is not defined in the DXF file. A line map will always use the selected color.
4. Check the check box next to the edit field. The map will be displayed only when the box is checked.

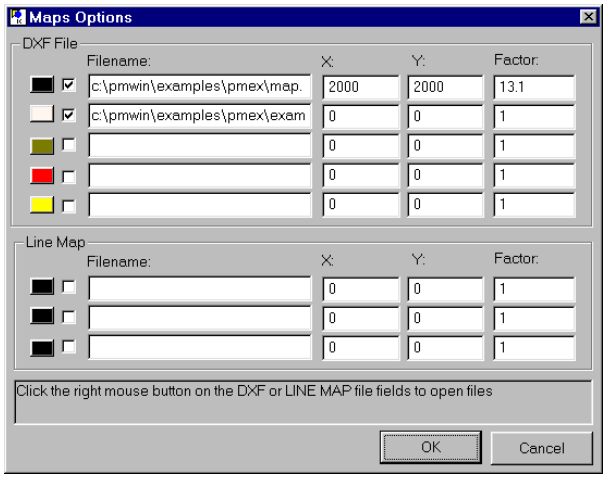


Fig. 4.12 The **Maps Options** dialog box

4.4 PMPATH Output Files

Plots

To create plot files, choose **Save Plot As...** from the **File** menu and specify the format and the file name in the **Save Plot As** dialog box (Fig. 4.13). Four formats are available: Drawing Interchange Format (DXF), Hewlett-Packard Graphics Language (HP-GL), Windows Bitmap (BMP) and the PATHLINE file of MODPATH 1.x. To select a format, click the Format drop-down box. You can type in the file name in the file edit field directly or click the right mouse button on the edit field and select a file from a **Plot File** dialog box.

Note that cross-sectional plots can only be included in the DXF and BMP-format. PMPATH uses the same color resolution as the video screen to capture and save Windows Bitmap files. The option **Use Polyline to save contours** should only be used if your graphics software accept the DXF entity POLYLINE.

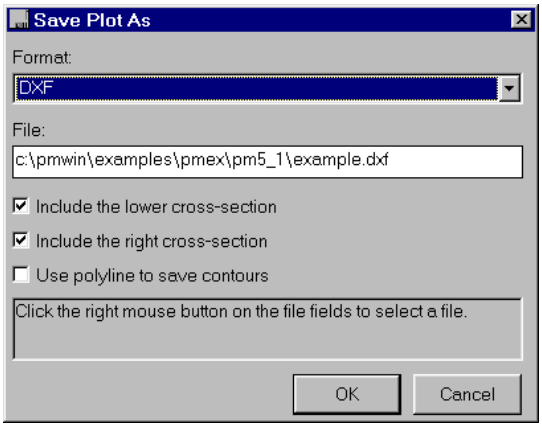


Fig. 4.13 The **Save Plot As** dialog box

If the MODPATH format is chosen, coordinates along the path of each particle are recorded in the file specified in the **Save Plot As** dialog box. The file contains the starting coordinates of a particle, and the coordinates at every point where a particle enters a new cell. In addition, coordinates of intermediate points are saved whenever a particle tracking step length is reached. The pathline file contains a sequence of one-line records, each line containing coordinate and location information for one point on a pathline. Each record contains nine variables, and is written using the FORTRAN-format

```
I5,1X,5(E20.12,1X),2(I3,1X),I3
```

The variables, in the order of appearance on the line, are defined as:

1. Particle index number: The index number is positive, if the forward particle tracking scheme is used. A negative index number indicates that the backward particle tracking scheme is used.
2. Global coordinate in the x-direction.
3. Global coordinate in the y-direction.
4. Verticle local coordinate within the cell
5. Global coordinate in the z-direction
6. Cumulative travel time.
7. J index of cell containing the point.
8. I index of cell containing the point.
9. K index of cell containing the point.

Except the particle index number, this format is identical to the PATHLINE FILE format described in the documentation of MODPATH.

Hydraulic heads

To save the hydraulic heads in the current layer at the current stress period and time step, select **Save Heads As...** from the **File** menu. PMPATH saves the hydraulic heads in ASCII Matrix format (see Appendix 2).

Drawdowns

To save drawdowns in the current layer, choose **Save Drawdowns As...** from the **File** menu and specify a file name in the standard File Save As dialog box. This menu item is disabled, if the drawdown file DDOWN.DAT is not available. PMPATH saves the drawdowns in the ASCII Matrix format (see Appendix 2).

Flow velocities

To save flow velocities in the current layer, choose **Save Velocity As...** from the **File** menu and specify a file name in the standard File Save As dialog box. Average pore velocities at the center of each cell are saved in the ASCII Matrix format (see Appendix 2). In addition, the velocity components along the I-, J- and K-axes are added to the end of the file. The default velocity at inactive cells is 1.0×10^{30}.

Particles

To save the position and the attributes of each particle, choose **Save Particles As** from the **File** menu and specify a file name in a **Save Particle As** dialog box. By selecting a file type in this dialog box, you can save either the starting position or end position (after backward or forward tracking) of each particle.

The following data format is used to save the particles:

1. Data: version label
2. Data: NP
3. Data: LI, LJ, LK, I, J, K, Z, C, R

The first line of this particle file contains the version label **PMPATH_V100_PARTICLES**. The second line contains the number of particles NP. The third record contains one line of data for each particle. The particle locations within the cell [J, I, K] are specified using local coordinates [LJ, LI, LK]. Local coordinates vary within a cell from zero to one as shown in Fig. 4.14. In addition, the global vertical coordinate Z, the color C and the retardation factor R of the particle are saved in the same line.

The particles file can be loaded by choosing **Load Particles** from the **File** menu. When you load a particle file, PMPATH just adds particles to the model. Already existing particles will not be removed.

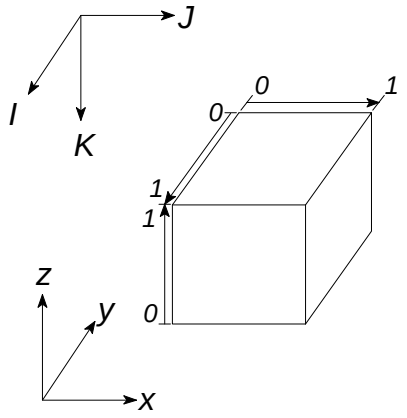


Fig. 4.14: Local coordinates within a cell

FOR YOUR NOTES

5. Modeling Tools

5.1 The Digitizer

To activate the digitizer, choose **Digitizer** from the **Tools** Menu. The **Digitizer** is based on the **Data Editor**. Using the **Digitizer** you can digitize, shift or delete points and assign a value to each of these points. An additional menu item **Points** in the **Value** menu allows you to delete all digitized points or save or load the points in or from an XYZ file. An XYZ file can be accepted by the **Field Interpolator** and has the following format:

N	first line of the file; N is the number of digitized points; The maximum allowed number is 10,000.
X_1, Y_1, Z_1	second line of the file
X_2, Y_2, Z_2	third line of the file
.	
.	
X_i, Y_i, Z_i	(i+1)-th line of the file
.	
.	
X_N, Y_N, Z_N	last line of the file

- **To digitize a point**

1. Click the **Digitize** button 
   You don't need to click the icon if its relief is already sunken.
2. Click the mouse cursor on the desired position to set a point.

- **To shift a digitized point**

1. Click the **Digitize** button 
2. Point the mouse cursor to a digitized point, holding down the left mouse button while moving the mouse.
3. Release the mouse button when the point is moved to the desired position.

- **To delete a digitized point**

1. Click the **Digitize** button 
2. Hold down the Ctrl-key and click the mouse cursor on a point.

▸ **To assign a value to a digitized point**

1. Click the **Digitize** button 
2. Move the mouse cursor to a point.
3. Press the right mouse button once.
   The **Digitizer** shows a dialog box.
4. In the dialog box, type a new value then click **OK**.

5.2 The Field Interpolator

Numerical groundwater models require areally distributed parameters (e.g. hydraulic conductivity, hydraulic heads, elevations of geological layers etc.) assigned to each cell or element in the model domain. Usually, the modeler obtains a parameter distribution in the form of scattered (irregular) data points (x_i, y_i, f_i), i=1, ..., N. N is the number of measurement points, x_i and y_i are the coordinates and f_i is the parameter value at point i. A basic problem is how to estimate the parameter values for each model cell from these data.

A number of interpolation (or extrapolation) methods for solving this kind of problems have been proposed. Some of the methods are used by commercial contouring software, e.g. GEOKRIG, GRIDZO, SURFER® or TECKON^{EM}. A common approach done by many modeler is that contour maps are firstly created by these software then overlaid on the model grid for assigning parameter values to model cells. The process is indirect and somewhat cumbersome.

The **Field Interpolator** provides a more direct way for assigning cell values by using the Kriging method and methods developed by Shepard (1968), Akima (1978a, 1978b) and Renka (1984a, 1984b). The interpolation programs take measurement data and interpolate the data to each model cell. The model grid can be irregularly spaced. Interpolation results are saved in the ASCII Matrix format (see Appendix 2), which can be accepted by the **Data Editor**. Depending on the interpolation method and the interpolation parameters the results may be slightly different. With the **Data Editor**, you can create contour maps of the interpolation results and visually choose a "best" result.

Theory is not emphasized in this description, because it is introduced in an extensive literature. For example, Watson (1992) presents a guide to the analysis and display of spatial data, including several interpolation methods. Franke (1982) provides a brief review and classification of 32 algorithms. Hoschek and Lasser (1992) give a comprehensive discussion of theories in geometrical data processing and extensive references in the area of data interpolation and

computer graphics techniques. Akin and Siemes (1988) and Davis (1973) provide necessary mathematical background skills on the statistics and data analysis in geology.

Starting the Field Interpolator

The **Field Interpolator** runs independently from PMWIN. To start the program, select **Field Interpolator** from the **Tools** menu of PMWIN or use the **Start** button on the task bar in Windows. The available settings of the **Field Interpolator** (Fig. 5.1) are grouped under three tabs - Files, Grid Position and Search/Gridding Method. These tabs are described below.

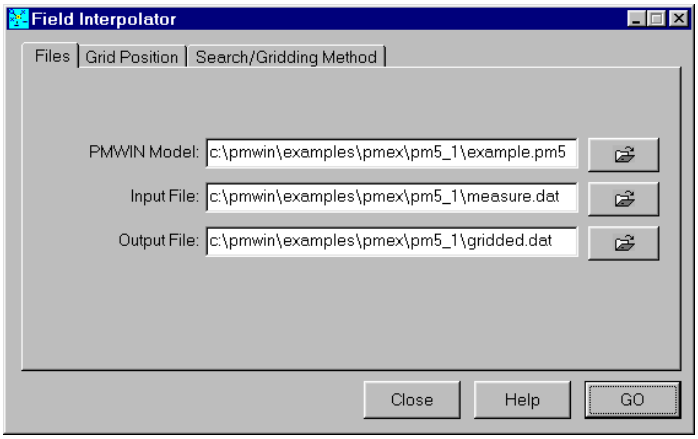


Fig. 5.1 The **Field Interpolator** dialog box

- **Files:**
  - **PMWIN Model**: If you have already opened a model within PMWIN and started the **Field Interpolator** from the **Tools** menu, this field contains the model file name. If "Open a model first" is shown, you must click  and select an PMWIN-model from a standard **Open File** dialog box. A PMWIN-model file always has the extension **.PM5**.
  - **Input File**: An input file contains the measurement data and can be prepared with the **Digitizer** or other software. Click  to select an existing input file. An input file must be saved in ASCII and have the following format:

N	first line of the file; N is the number of data points;
X_1, Y_1, Z_1	second line of the file
X_2, Y_2, Z_2	third line of the file
.	
X_i, Y_i, Z_i	(i+1)-th line of the file
.	
.	
X_N, Y_N, Z_N	last line of the file

Where N is the number of data points, x_i and y_i are the x- and y-coordinates of data point i and f_i is the measurement value at data point i. **The maximum number of data points is 2000.**

- **Output file**: An output file contains the interpolated data for each model cell and is saved in the ASCII matrix format. See Appendix 2 for the format of the ASCII matrix file.

- **Grid Position**:

Using the rotation angle and the coordinates (X_0, Y_0) of the left corner of the model grid, you may rotate and place the grid at any position. The rotation angle is expressed in degrees and is measured counterclockwise from the positive x-direction. See section 3.9 for details about the coordinate system of PMWIN. As we normally define the grid position and the coordinate system at the beginning of a modeling process, the grid position will rarely be changed here.

- **Gridding Method**:

PMWIN provides four gridding methods, namely Shepard's inverse distance method, Akima's bivariate interpolation method, Renka's triangulation method and the Kriging method. You can select a method from the drop-down box. For each gridding method, there is a corresponding interpolation program. The interpolation programs are written in FORTRAN and were compiled with a 32-bit compiler.

- **Shepard's inverse distance**: The Shepard's inverse distance method uses eq. 5.1 to interpolate data for finite-difference cells.

$$f = \frac{\sum_{i=1}^{N} [\, f_i / (\, d_i^F)]}{\sum_{i=1}^{N} [\, 1 / d_i^F]} \qquad (5.1)$$

Where d_i is the distance between data point i and the center of a model cell, f_i is the value at the i-th data point, F is the weighting exponent and f is the estimated value at the model cell.

The weighting exponent must be greater than zero and less than or equal to 10. Fig. 5.2 shows the effects of different weighting exponents. Five data points are regularly distributed along the x-axis. Using higher values for the exponent (e.g., F = 4) the interpolated cell values will approach the value of the nearest data point. The surface is therefore relatively flat near all data points. Lower values of the exponent (e.g. F = 1) produce a surface with peaks to attain the proper values at the data points. A value of F = 2 is suggested by Shepard (1968).

- **Akima's bivariate interpolation:** This method creates a triangulation of the measurement data points and performs interpolation by using a bivariate fifth order polynomial of Hermite type for the interpolation within a triangle. It uses a user-specified number of data points closest to a model cell for estimating the value at the cell.
- **Renka's triangulation:** This method creates a triangulation of the measurement data points and uses a global derivative-estimation procedure to compute estimated partial derivatives at each point. The program determines a piecewise cubic function F(x,y). F has continuous first derivates over the created mesh and extends beyond the mesh boundary allowing extrapolation.

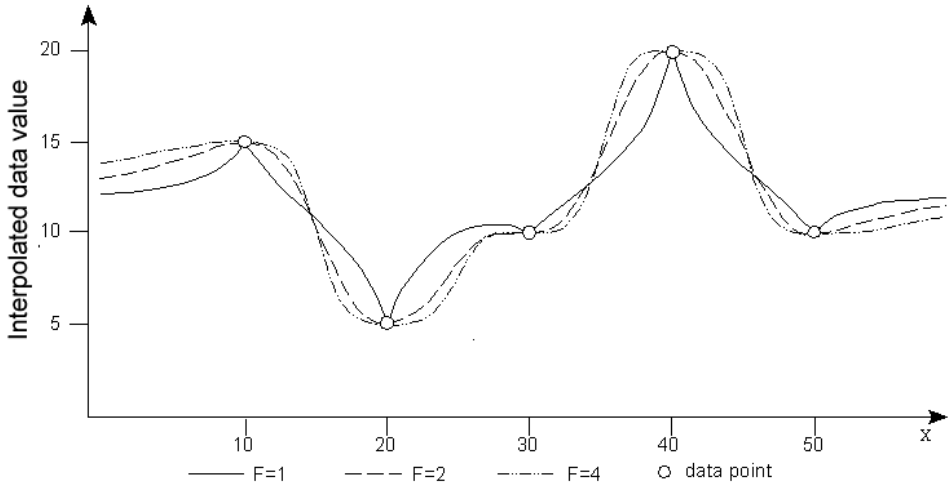


Fig. 5.2 Effects of different weighting exponents

- **Kriging:** The Kriging method has been popularized by Mathéron (1963) and is named in honor of D. G. Krige, a noted South African mining geologist and statistician. PMWIN assumes that the measurement data are stationary and isotropic. The Kriging method estimates the value at a model cell from a user-specified number of adjacent data values while considering the interdependence expressed in the variogram.

  A variogram is a plot of semivariance $\gamma_{(h)}$ versus vector distance **h**. The variogram is used to define the relationship of the measurement values or to estimate the distance over which measurement values are interdependent. When you select **Kriging** as the gridding method, a **Variogram** appears. Click this button to display the Variogram dialog box (Fig. 5.3). You need to select a variogram model from the drop-down box and specify the parameters for the selected variogram model. PMWIN does not provide a procedure for fitting the selected variogram curve to the measurement data. This is a task for geostatistical software, e.g., VarioWin (Y. Pannatier, 1996) or GEO-EAS (E. Englund and A. Sparks, 1991) by the US-

EPA, and beyond the objective of this software. If you do not know the variogram type, use the linear variogram. Kriging with a linear variogram is usually quite effective.

The meaning of necessary parameters and the equations used by the programs are listed below:

- Power law and linear model:

$$\gamma_{(h)} = \alpha \cdot |h|^{\omega} + c_0 \qquad \alpha>0,\ 0<\omega<2 \qquad (5.2)$$

- Logarithmic model

$$\gamma_{(h)} = 3\alpha \cdot \log|h| + c_0 \qquad \alpha>0 \qquad (5.3)$$

- Spherical model

$$\gamma_{(h)} = C \cdot \left(\frac{3}{2} \cdot \frac{|h|}{a} - \frac{|h|^3}{2a^3}\right) + c_0 \qquad h \le a$$
$$\gamma_{(h)} = C + c_0 \qquad h>a \qquad (5.4)$$

- Gaussian model

$$\gamma_{(h)} = C \cdot (1 - EXP[-h^2/a^2]) + c_0 \qquad (5.5)$$

- Exponential model

$$\gamma_{(h)} = C \cdot (1 - EXP[-|h|/a]) + c_0 \qquad (5.6)$$

Where C is the variance of measurement data and will automatically be calculated by the program, a the correlation length, c_0 the nugget variance, α the slope and ω the power factor of the power model. ω=1 yields the linear model (Fig. 5.4). The variance C will be calculated by the program.

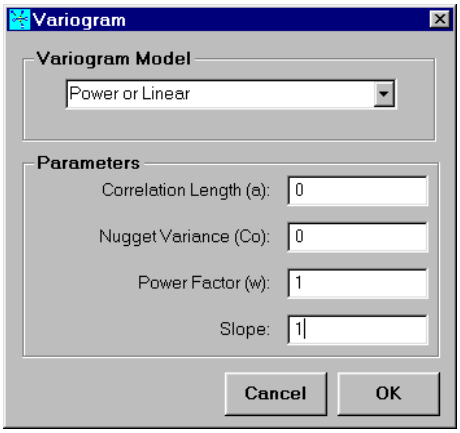


Fig. 5.3 The **Variogram** dialog box

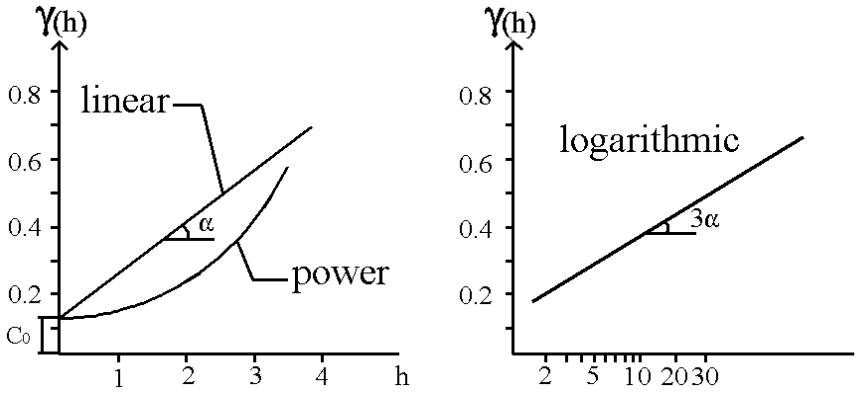


Fig. 5.4 Linear, power and logarithmic model

- **Search Method**:

  The interpolation algorithms use three search methods to find a certain number of the measurement data points to interpolate a cell value. The search methods are called **SIMPLE**, **QUADRANT** and **OCTANT**. The search radius is assumed to be infinitely large.

  The **SIMPLE** search method finds the data points nearest to the model cell. The **QUADRANT** or **OCTANT** search methods find closest data points from each quadrant or octant around a model cell (Fig. 5.5a and 5.5b). The number of data points used in a search is defined by the **Data Per Sector** value. If fewer than **Data Per Sector** points are found in a sector, the program uses the other nearest points found in the entire model. The valid range of **Data Per Sector** is

SIMPLE	$3 \leq$ **Data Per Sector** ≤ 30
QUADRANT	$1 \leq$ **Data Per Sector** ≤ 7
OCTANT	$1 \leq$ **Data Per Sector** ≤ 3

  The search method defaults to **OCTANT** search. Octant or quadrant searches are usually used when the measurement points are grouped in clusters. These search methods force the interpolation programs to use measurement data points radially distributed around the model cell. They usually introduce more smoothing than a **SIMPLE** search.

  Note that the entries in Search Method are ignored when Renka's triangulation algorithm is used.

- **GO**:

  To start the interpolation, simply click the button **GO**. The field generator creates and writes the settings and the coordinates to a batch file PMDIS.BAT and two ASCII files PMDIS_IN.{1} and PMDIS_IN.{2}. After having created these files, PMDIS.BAT will be run in a DOS-window. The created ASCII files are used by the interpolation program.

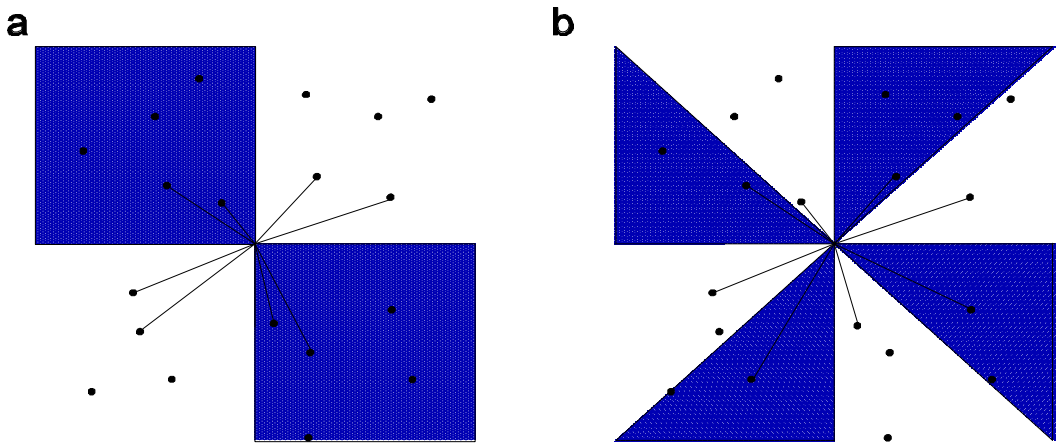


Fig. 5.5 Search pattern used by (a) Quadrant Search (**Data Per Sector**=2) and (b) Octant Search (**Data Per Sector**=1)

5.3 The Field Generator

The **Field Generator** (Frenzel, 1995) can generate fields with heterogeneously-distributed transmissivity or hydraulic conductivity. This allows the user to do stochastic modeling with PMWIN. In stochastic modeling, uncertainty due to unknown small-scale variability of the model parameters is addressed directly by assuming that the parameters are random variables. Hydraulic conductivity or transmissitivity is commonly assumed to be lognormally distributed. We denote the hydraulic conductivity by X and a variable Y=log(X). When Y is normally distributed with a mean value μ and standard deviation σ, then X has a lognormal distribution.

Starting the Field Generator

The **Field Generator** runs independently from PMWIN. To start the program, select **Field Generator** from the **Tools** menu of PMWIN or use the **Start** button on the task bar in Windows. A dialog box appears (Fig. 5.6). The program uses the correlation scales in both I and J-directions and the mean value μ and standard deviation σ of log-transformed measurement values to generate a quantitative description (a realization) of the hydraulic conductivity or transmissivity field. The size of the field (number of cells) and the number of desired realizations is specified in the dialog box. Realizations are saved in the ASCII Matrix format (see Appendix 2) using the file names *filename.xxx*, where *filename* is the output file name specified in the dialog and *xxx* is the

realization number. Note that *filename* should not be the same as the name of your model, because PMWIN uses the same convention to save some internal data files.

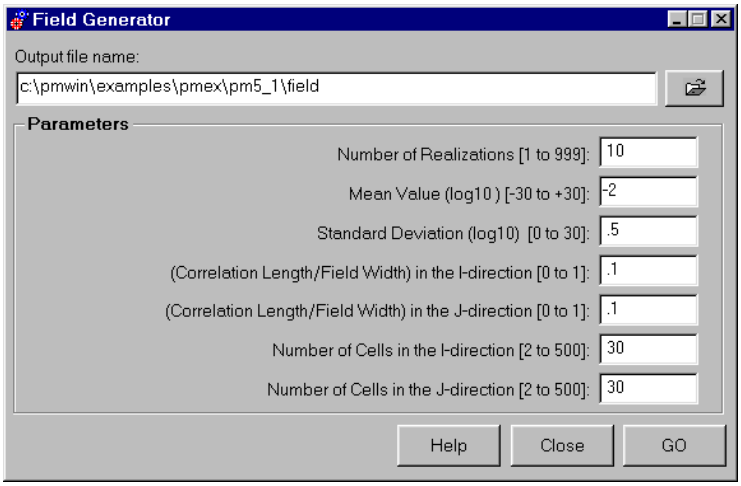


Fig. 5.6 The **Field Generator** dialog box

The generated field is lognormally (to base 10) distributed. Using the **Data Editor**, you can load the generated field into an area of the model grid where the columns and rows are regularly spaced (see section 3.8 for how to load an ASCII matrix file). The simulation of the hydraulic conductivity distribution produced in this way is unconditional because the hydraulic conductivity values are not constrained to match the measurement values. In conditional simulation existing measurements are used which reduce the space of possible realizations. The conditional generation of a single realization proceeds in five steps:

1. The parameter value for each model cell is interpolated from the measurements using the Kriging method. The correlation length is determined from the measurements.
2. An unconditional generation is performed using the Field Generator with the same correlation length (correlation scale).
3. The unconditionally generated values at the measurement locations are used to interpolate values for each model cell by using the Kriging method again.
4. The distribution from step 3 is subtracted from the distribution from step 2 yielding kriging-residuals.
5. The kriging-residuals are added to the distribution from step 1 yielding a realization which has the same correlation length and passes through the measured values at the measurement points.

5.4 The Results Extractor

Normally, simulation results from MODFLOW, MT3D or MT3DMS are saved unformatted (binary) and cannot be examined by using usual text editors. Using the **Results Extractor**, you may extract specific results from the result files and save them in ASCII Matrix or Surfer Data files (see Appendix 2 for the format).

There are two ways to start the **Result Extrator**. If you are in the main menu of PMWIN, select **Result Extractor...** from the **Tools** menu. If you are using the **Data Editor,** select **Result Extractor...** from the **Value** menu. The **Result Extractor** dialog box (Fig. 5.7) contains a spreadsheet, an **Orientation** drop-down box, a **Layer** edit field, a **Column Width** drop-down box, four tabs and several command buttons. They are described below.

- **Spreadsheet**: The spreadsheet displays a series of columns and rows, which correspond to the columns and rows of the finite-difference grid. By clicking the **Read** button, the selected result type will be read and put into the spreadsheet.
- **Orientation** and **Layer**: Simulation results can be loaded layer-, column- or row-wise. **Orientation** decides how the results should be loaded. If the orientation is **Plan View**, you are asked to enter a layer number into the edit field. If **X-section (column)** or **X-section (row)** is selected, you should enter a column or row number into the edit field next to drop-down box.
- **Column Width:** This drop-down box is used to change the appearance width of the columns of the speadsheet.
- **Tabs**: Each tab corresponds to a simulation model. The tabs are described below.
  - **MODFLOW**: The result files of MODFLOW include hydraulic head, drawdown, preconsolidation head, compaction, subsidence and cell-by-cell flow terms (see **MODFLOW▸Output Control** of section 3.6.1 for the definition of each term). You can choose a result type from the **Result Type** drop-down dox. The stress period and time step, from which the result is read, are given in the corresponding edit fileds.
  - **MOC3D**: The result files of MOC3D include concentration and velocity terms. You can choose a result type from the **Result Type** drop-down dox. The simulation time, from which the result is read, can be selected from the **Total Elapsed Time** drop-down box. This drop-down box is empty, if the selected simulation result does not exist.
  - **MT3D**: The primary result of MT3D is concentration. If you are using MT3D96, two additional result types, i.e. solute mass and sorbed mass, can be selected. The simulation time, from which the result is read, can be selected from the **Total Elapsed Time** drop-down box. This drop-down box is empty, if the selected simulation result does not exist.

  - **MT3DMS**: The primary result of MT3DMS is concentration. The species number and simulation time, from which the result is read, can be selected from the **Species Number** and **Total Elapsed Time** drop-down boxes. These drop-down boxes are empty, if simulation results do not exist.
- **Save...** and **Read**: To extract a certain result type, simply click the **Read** button. You may save the contents of the spreadsheet by clicking the **Save...** button and specifying the file name and the file type in a **Save Matrix As...** dialog box. There are four file types, *ASCII Matrix (Warp form)*, *ASCII Matrix*, *SURFER files* and *SURFER files (real-world).* An *ASCII Matrix* file may be loaded into the spreadsheet at a later time. The format of the ASCII matrix file is described in Appendix 2. A SURFER file has three columns containing the (x, y) coordinates and the value of each cell. If the file type is *SURFER files*, the origin of the coordinate system for saving the file is set at the lower-left corner of the model grid. If the file type is *SURFER files (real-world)*, the real-world coordinates of each cell will be saved. The real-world coordinate system is defined by **Options ▸ Environment** (section 3.9)**.**
- **Apply**: The **Apply** button appears only if you start the **Result Extractor** from the **Data Editor** via **Value▸Result Extractor...**. Click on this button, the content of the spreadsheet will be put into the model grid. Note that this button is dimmed (and cannot be used), if the spreadsheet is empty or the orientation is not **Plan View** or the data has been applied to the model grid.

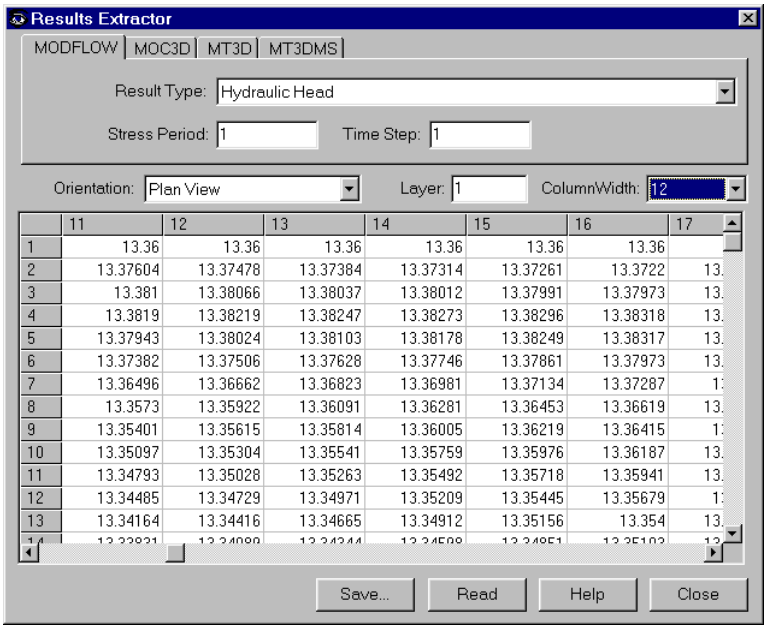


Fig. 5.7 The **Results Extractor** dialog box

5.5 The Water Budget Calculator

There are situations in which it is useful to calculate flow terms for various subregions of the model. To facilitate such calculations, the computed flow terms for individual cells are saved in the file BUDGET.DAT. These individual cell flows are referred to as cell-by-cell flow terms, and are of four types: (1) cell-by-cell stress flows, or flows into or from an individual cell due to one of the external stresses (excitations) represented in the model, e.g., pumping well or recharge; (2) cell-by-cell storage terms, which give the rate of accumulation or depletion of storage in an individual cell; (3) cell-by-cell constant-head flow terms, which give the net flow to or from individual constant-head cells; and (4) internal cell-by-cell flows, which are the flows across individual cell faces. In the file BUDGET.DAT, the flow between the cells [J, I, K] and [J+1, I, K] is denoted by FLOW RIGHT FACE, the flow between the cells [J, I, K] and [J, I+1, K] is denoted by FLOW FRONT FACE, and the flow between the cells [J, I, K] and [J, I, K+1] is FLOW LOWER FACE. The Water Budget Calculator uses the cell-by-cell flow terms to compute water budgets for the entire model, user-specified subregions, and in- and outflows between adjacent subregions. Refer to **Step 5: Calculate subregional water budget** of Section 2.1 for details.

5.6 The Graph Viewer

To activate the graph viewer, select an appropriate menu item from the **Run▸Graphs** menu. The Graph Viewer (Fig. 5.8) allows you to examine temporal development curves of the observations and the simulation results, including hydraulic heads, drawdowns, concentration, preconsolidation heads, compaction of each model layer and subsidence of an entire aquifer. (Note that drawdown is defined by $h_0 - h$, where h_0 is the starting hydraulic head and h is the calculated head at time t.) The coordinates of boreholes and the corresponding observed data are specified in the **Boreholes and Observations** dialog box (see section 3.5).

PMWIN uses a bilinear interpolation scheme to calculate values at user-specified boreholes. For each user-specified borehole, the values of the four model cells surrounding that borehole are determined first. The simulation results at those cells are then interpolated to obtain the value at the borehole by using the following equation:

$$h = \frac{\Sigma(h_i \cdot A_i)}{\Sigma A_i} \qquad i = 1 \text{ to } 4; \quad A_i = 0 \text{ if } h_i = HDRY, HNOFLO \text{ or } CINACT \qquad (5.7)$$

where A_i is the area and h_i is the computed value at the center of a cell as shown in Fig. 5.9; HNOFLO and HDRY are predefined heads for no-flow cells and dry cells, and CINACT is the predefined concentration value for inactive concentration cells. If a borehole lies in an inactive cell, h=HDRY.

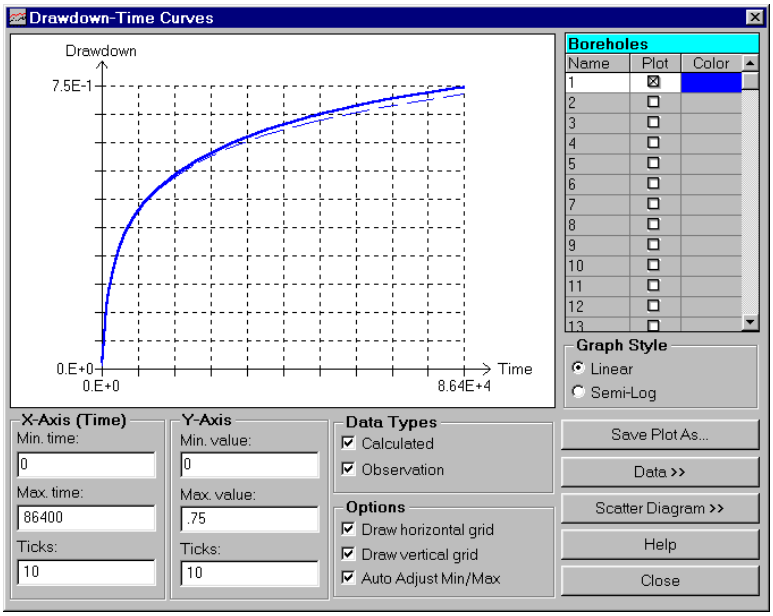


Fig. 5.8 The Graph Viewer displaying drawdown-time curves

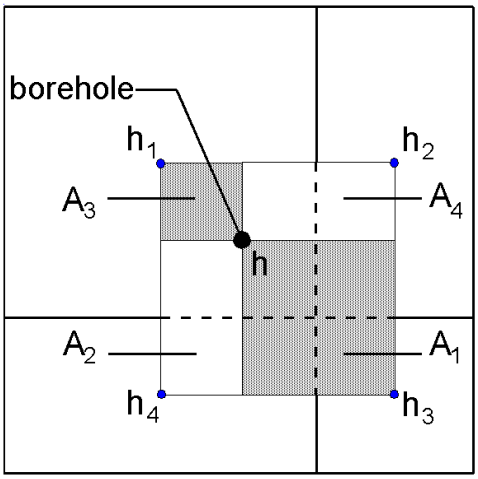


Fig. 5.9 Interpolation of simulation results to a user-specified borehole

The available settings of the **Graph Viewer** are summarized below.

- **The Borehole table:** The table contains the borehole numbers and the plot colors. The curve of a borehole will be displayed only when the corresponding **Plot** flag is checked. The plot color of each curve is given in the **Color** column. Click on a colored cell of the table to

change the color. Note that if you have deactivated a borehole in the Boreholes and Observations dialog box, the corresponding row of the table is dimmed and its settings cannot be changed.

- **X-Axis (Time): Min. Time** and **Max. Time** define a range of simulation time for which the curves should be displayed. The number of desired ticks is given in the edit field **Ticks**.
- **Y-Axis: Min. Value** and **Max. Value** specify the minimum Y-axis value and maximum Y-axis value on the graph. The number of desired ticks is given in the edit field **Ticks**.
- **Data Types**: Check the **Calculated** or **Observation** box to display the curves based on the computed or observed data. The graph viewer uses solid lines for displaying calculated curves. Observation curves are dashed.
- **Options:** Check the **Draw Horizontal Grid** or **Draw Vertical Grid** box to display the reference grids on the graph. If **Auto Adjust Min/Max** is checked, the graph viewer uses the minimum and maximum simulation times and values from the simulation result.
- **Graph Style:** You can display the time axis (X-axis) either on a linear or logarithmic scale.
- **Save Plot As:** Use this button to save the graph in Windows bitmap format.
- **Data »**: Click this button to display the **Value Tables** dialog box (Fig. 5.10) showing the observed and calculated values at active boreholes. You can save the calculated values in an ASCII data file or in the Observation file format (see Appendix 2 for the format) by clicking the **Save As...** button. Data saved in the Obervation file format can be imported into the **Observation** table of the **Boreholes and Observations** dialog box (see section 3.5).
- **Scatter Diagramm »**: Click the button to display the **Scatter diagram** dialog box (Fig. 5.11). Scatter diagrams are often used to present the quality of calibration results. The observed values are plotted on one axis against the corresponding calculated values on the other. If there is exact agreement between measurement and simulation, all points lie on a 45° line. The narrower the area of scatter around this line, the better is the match.

  Note that a borehole will be displayed and used for calculating the variance (between observed and calculated values) only when the corresponding **Plot** flag in the **Borehole table** is checked. You can edit the text on the scatter diagram by clicking the mouse on the desired text. Clicking on the **Save Plot As**, you can save the plot in the Windows BMP format. The other options are self-explanatory.

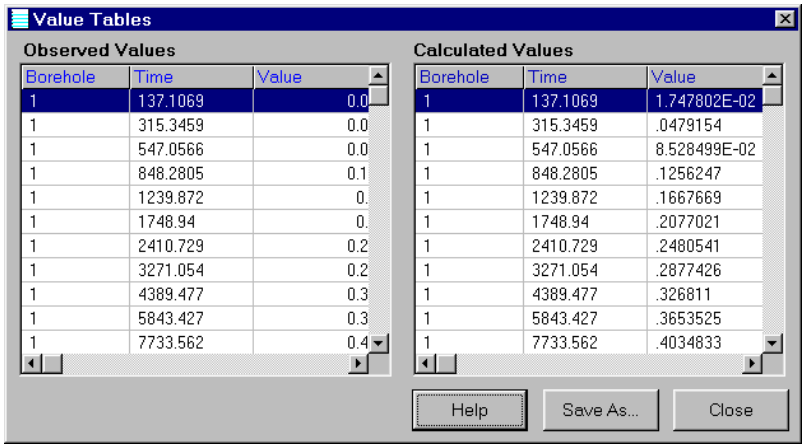


Fig. 5.10 The **Value Tables** dialog box

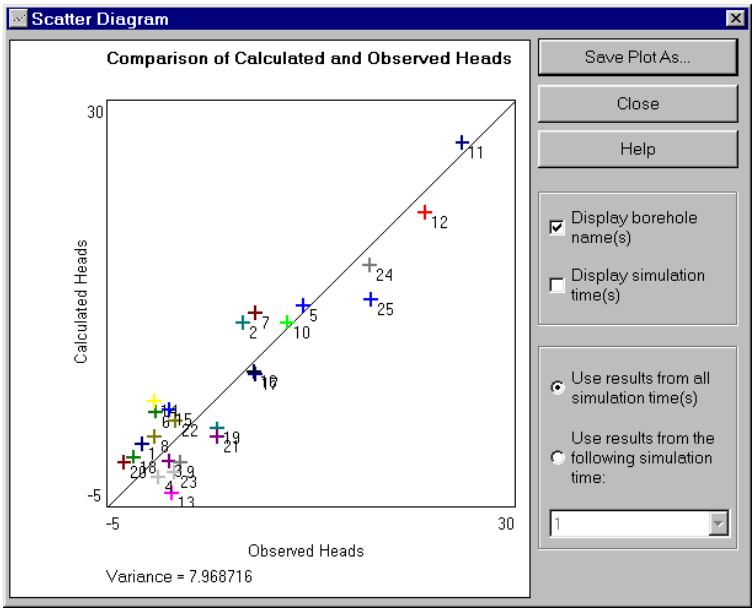


Fig. 5.11 The **Scatter Diagramm** dialog box

FOR YOUR NOTES

6. Examples and Applications

The sample problems contained in this chapter are intended to illustrate the use of PMWIN and the supported programs. The sample problems are described in the following sections. Each section deals with a specific theme. The models of each section can optionally be installed during the installation of PMWIN. Except the tutorials, the description of each problem is divided into three parts. It starts out with **Folder**, where you can find the ready-to-run model, for example \pm5\examples\tutorials\tutorial1\. Next, you'll find a discussion of the problem and finally you will find the simulation results. Note that you should change the path \pm5\, if you have installed PMWIN in an other folder.

6.1 Tutorials

6.1.1 Tutorial 1 - Unconfined Aquifer System with Recharge

Folder: \pm5\examples\tutorials\tutorial1\

Overview of the Problem

This simple scenario is designed to demonstrate the basic features of PMWIN and MODFLOW. An unconfined aquifer (Fig. 6.1) is a coarse grained sand with a measured isotropic hydraulic conductivity of 160 m/day, the specific yield has been assessed as 0.06. Recharge to the aquifer only occurs throughout the 4 month wet season at a rate of 7.5×10^{-4} m/day, outside the wet season there is no recharge to the aquifer. The elevations of the aquifer top and bottom are 25 m and 0 m, respectively. The area of interest is 10000 m long and 6000 m wide and is bounded by "no flow" zones to the east and west. There is also a volcanic mountain in the south east corner of the model area. To the north an area of constant hydraulic head existd with a value of 15 m. The southern boundary is a specified flux boundary with an inflow rate of 0.0672 m^3/day per meter. A total of nine wells in the area are pumped at 45 l/s (3888 m^3/d) each during the 8 month dry season to supply water for irrigation and domestic purposes.

Your task is to assess the water levels in the aquifer under the following conditions:

1. steady-state, with the mean recharge rate = 2.5×10^{-4} m/day, no pumping;
2. after 8 months pumping during the dry season; and
3. the water levels by the end of the following wet season.

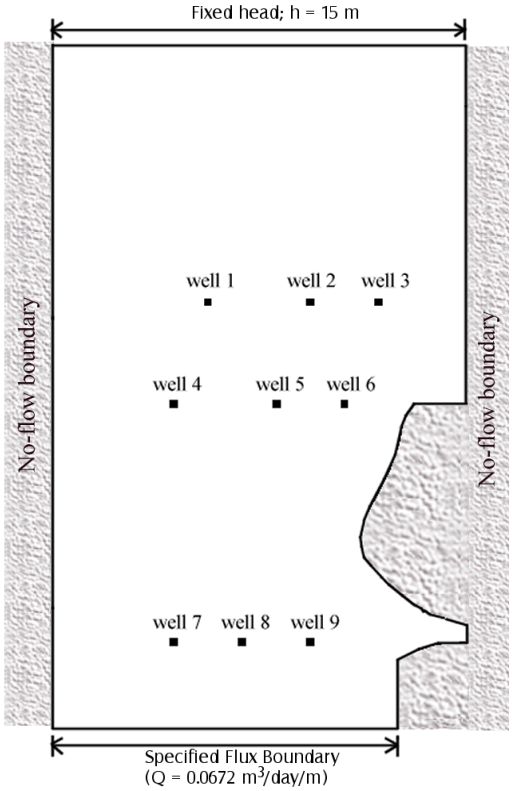


Fig. 6.1 Plan view of the model area

There are eight main steps in this tutorial:

1. Create a new model,
2. Define model size,
3. Refine model grid,
4. Assign model data,
5. Perform steady-state flow simulation,
6. Extract and view results from the steady-state simulation,
7. Produce output from the steady-state simulation, and
8. Transient flow simulation.

This tutorial will lead you through the steps required to construct a working groundwater model of the area being studied and to then use the model to assess the effects of changing some parameters on the modelled results. Instructions are given for each step of the process in the following manner:

- Select items from the menu: in **BOLD**
- A series of commands: linked by ▸

for example to open a new model the steps are **File ▸ New Model …**

Step1: Create a New Model

- **To create a new model,**

1. Select **File ▸ New Model …**
2. In the **New Model** dialog box, change the working folder to \pm5\examples\T1 (create the folder, if it does not exist) and enter T1 as the name of the new model to be created.
3. Click **OK** to exit this dialog box.

Step 2: Define Model Size

- **To define the size of the model**

1. Select **Grid ▸ Mesh Size...**
2. In the **Model Dimension** dialog box enter,

Layers	Number	1
Columns	Number	12
	Size	500
Rows	Number	20
	Size	500

3. Click **OK** to exit this dialog box.

You are now in the **Grid Editor** of PMWIN. To help visualize the problem we can overlay a DXF file as a map, which gives us the locations of the boundaries and the pumping wells.

- **To load a map**

1. Select **Options ▸ Maps…** to open the **Map Options** dialog box.
2. Click the box beside the space for the DXF filename to activate that particular map (it is also possible to choose a color by clicking on the colored square).
3. In the first filename field of DXF-files, click the right mouse button to bring up the **Map Files** dialog box.
4. Choose BASEMAP1.DXF from the folder \pm5\examples\tutorials\tutorial1\, click **OK** to exit the dialog box.

5 Click **OK** to exit the **Map Options** dialog box.

Step 3: Refine Model Grid

It is good practice to use a smaller grid in areas where the hydraulic gradient is expected to be large, in this case it is around the wells. In PMWIN, grid refinement takes place within the **Grid**

▸ **Mesh Size…** and it is quite easy to add additional rows and columns to an existing mesh. This is done by using a combination of holding down the CTRL key and using the arrow keys as follows:

CTRL + Up arrow - add a row
CTRL + Down arrow - remove an added row
CTRL + Right arrow - add a column
CTRL + Left arrow - remove an added column.

It is also possible to specify the row and column spacing of individual cells by clicking the right mouse button within the cell of interest, however we will not be doing that in this exercise.

▸ **To refine the mesh around the pumping wells**

1. If you aren't already in the **Grid Editor**, enter by
   Grid ▸ Mesh Size…
2. Zoom in around Well 1 by clicking on the button and then dragging a box around the general area of Well 1.
3. Change back to the button and click on the cell containing Well 1.
4. Divide this column into three by adding two additional columns
   CTRL + Right arrow followed by
   CTRL + Right arrow
5. Divide the row also into three by
   CTRL + Up arrow followed by
   CTRL + Up arrow
   You should see dashed lines where the new rows and columns will be placed.
6. Zoom out by pressing the button. You will notice that the rows and columns added extend throughout the model domain and form part of the fine discretisation around some of the other wells.
7. Repeat the above refinement around Well 2 to Well 9, remember some of the discretisation has already been done when you added rows and columns around Well 1.
8. At this stage your cells increase from a size of 167 m to 500 m abruptly, in order to have a more gradual increase in cell size we need to half the size of the following rows and columns (again using the CTRL key and the arrow keys).
   Columns 3 and 11
   Rows 7, 9, 10, 12, 17, and 19
   The number of the rows and columns are given in the status bar on the bottom of the screen and are numbered such that the cell specified by Column 1, Row 1 is the top left cell of the model (in a 3D sense the top layer is also Layer 1 with Layer numbers increasing with

depth). Upon completion of the refinement your grid should look like that in Fig. 6.2.

9. Leave the **Grid Editor** by **File ▸ Leave Editor ▸ Yes**

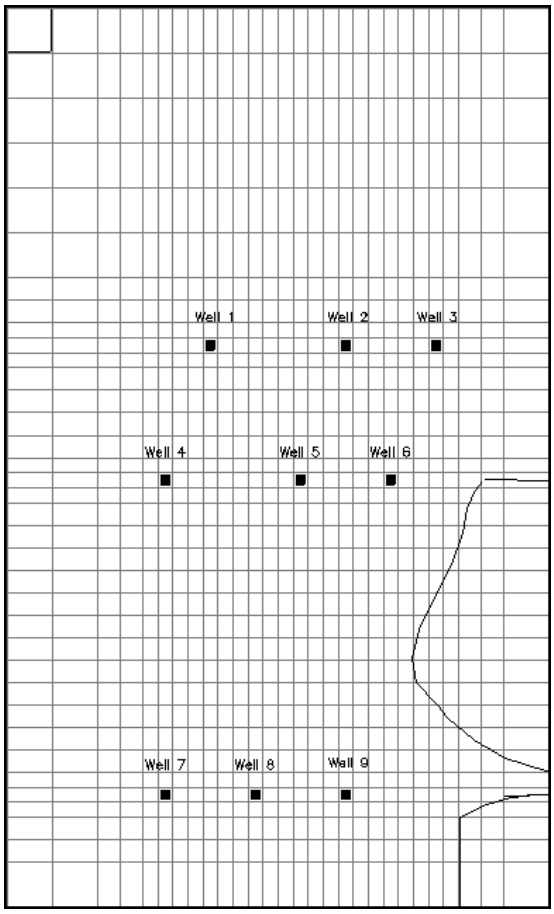


Fig. 6.2 Model discretization

Step 4: Assign Model Data

The **Data Editor** is accessed each time some spatial data (such as recharge, hydraulic conductivity etc.) need to be input to the model. The format and commands of the **Data Editor** are the same for each parameter and once you become familiar with the commands and menus it is very easy to enter and change the model data. The values of the particular data being edited or entered and the selected cell are displayed in the status bar on the bottom of the screen.

The model data for the task #1 (steady-state water level, with recharge, no pumping) includes **aquifer types, flow boundaries, aquifer geometry, aquifer parameters, initial conditions, time paramters** and **recharge rates**.

Aquifer types

Since we only have one layer in the model it is relatively straightforward to define it as unconfined.

▸ **To define the aquifer type**

1. Select **Grid ▸ Layer Type …**
2. In the **Layer Options** dialog box, click on Type and select Unconfined, it is okay to browse through the rest of this dialog box, but leave all the values as the default ones.
3. Click OK to leave the **Layer Options** dialog box.

Flow boundaries

MODFLOW uses an array called the IBOUND array to determine if a particular cell is active, inactive (no flow) or a fixed-head cell. Cell values within IBOUND are as follows:

active	=	1 (or other positive integers)
inactive	=	0
fixed-head	=	-1 (or other negative integers)

These values are assigned to cells as required in the **Data Editor**. By default and convention the area outside the model domain is deemed to be a "No Flow Zone" and as such it is not necessary to set this area to inactive.

▸ **To specify the IBOUND data**

1. Select **Grid ▸ Boundary Condition ▸ IBOUND (Modflow)**
2. Make sure the cell selected is [1,1,1] and click the right mouse button to open the **Cell Value** dialog box. Since this is going to be a fixed-head boundary enter -1, and click **OK** to exit the dialog box. The cell should now have a blue color signifying that it has been set as fixed-head.
   To save doing this for the remaining fixed-head cells it is possible to copy the value (in this case -1) to any other cell.
3. Click on the **Duplication** Button  , **duplication** is activated if the relief of the button is sunk.
4. Simply click the left mouse button in any cell that you want to specify as a fixed-head cell. If you make a mistake, turn off the **Duplication** Button and click the right mouse button in the cell where you have entered the wrong value and replace it with the desired value.

5. Complete specifying the entire North boundary as fixed-head cells. We will assign a head value to these cells a little later.

The outer grid boundaries are assigned as *No Flow* by default. However, the mountain area in the south corner of the domain, which is impervious and still falls inside the model grid, needs to be explicitly assigned as *No Flow* (ie. IBOUND=0).

▸ **To specify the no-flow zone**

1. Ensure **Duplication** is off and click in a cell within the *No Flow* zone.
2. Click the right mouse button to open the **Cell Value** dialog box.
3. Enter 0 as the value for IBOUND and click OK to exit the dialog box. You will notice that the cell is now gray in color.
4. Either repeat the above 3 steps for the remaining No Flow cells or turn on the **Duplication** and copy the value of IBOUND=0 to the other cells. In some cases you will notice that the boundary cuts through part of a cell. In these cases you need to make a judgement as to whether the cell should remain active (IBOUND=1) or be specified as inactive (IBOUND=0). Generally, you should choose the option which applies to more than 50% of the cell area. If all the steps were completed correctly, the grid should now look similar to that in Fig. 6.3.
5. Leave the Data Editor by **File ▸ Leave Editor ▸ Yes**

Aquifer geometry

The next step in the process is to specify the top and bottom elevations of each aquifer in the model. We need to set the aquifer top elevation to 25m and we can leave the elevation of the bottom of the aquifer as the default value of 0m.

▸ **To specify Aquifer Top**

1. Select **Grid ▸ Top of Layers (TOP)**
2. Since the aquifer top elevation is uniform throughout the model it is possible to set a single value to the entire grid by **Value ▸ Reset Matrix**...
3. Enter 25 in the **Reset Matrix** dialog box and click **OK** to exit.
4. Leave the Data Editor by **File ▸ Leave Editor ▸ Yes**

Repeat the above process to set the elevation of the base of the aquifer to 0m. Although the default value in this model is zero, we still have to enter the editor to let the model knows that

the parameter has been specified.

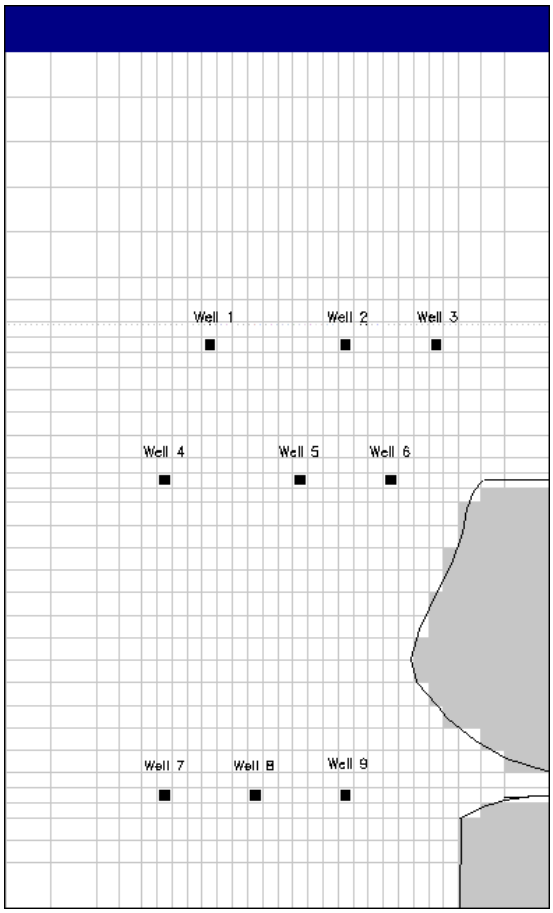


Fig. 6.3 Boundary conditions

Aquifer parameters

The next stage is to assign the aquifer parameters.

- **To specify the horizontal hydraulic conductivity**

1. Select **Parameters ▸ Horizontal Hydraulic Conductivity**
2. Since the horizontal hydraulic conductivity is uniform throughout the model it is possible to set a single value to the entire grid by **Value ▸ Reset Matrix**...
3. Enter 160 in the **Reset Matrix** dialog box and click **OK** to exit.
4. Leave the Data Editor by **File ▸ Leave Editor ▸ Yes**

Initial Conditions

MODFLOW requires some initial hydraulic head conditions to enable it to perform the flow simulation. In a steady state flow model only the hydraulic head values of the fixed-head cells are important as these do not change throughout the simulation. The values in the other cekks serve as initial guesses for the iterative solvers. In a transient simulation however, the hydraulic heads at the start of the simulation are the basis for determining the resulting head distribution after the aquifer is subject to some time-dependent stresses. It is usual to perform a steady state flow simulation first and use the resulting head distribution as the basis for the transient simulations, which is what we shall do in this case.

▸ **To set the initial hydraulic heads**

1. Select **Parameters ▸ Initial Hydraulic Heads**
2. Firstly set the entire grid to a uniform value by **Value ▸ Reset Matrix...**
3. Enter 16 in the **Reset Matrix** dialog box and click **OK** to exit.
4. Now set hydraulic head of the northern fixed-head boundary to 15 metres by first selecting the top left cell [1,1,1] with the left mouse button and then assigning a value of 15 by clicking with the right mouse button and entering 15 in the **Cell Value** dialog box.
5. Copy the value of 15 to the remainder of the northern boundary using the **Duplication** Button and the left mouse button.
6. Leave the **Data Editor** by **File ▸ Leave Editor ▸ Yes**

Time Parameters

▸ **To specify the time parameters**

1. Select **Parameters ▸ Time...**
2. In the **Time Parameters** dialog box, change the Simulation Time Unit to **DAYS** and check that **Steady-State** is selected in the **Simulation Flow Type** box.
3. Click **OK** to leave the **Time Parameters** dialog box.

Recharge rates

▸ **To specify the recharge rate**

1. Select **Models ▸ MODFLOW ▸ Recharge**
2. Set the entire grid to a uniform value by **Value ▸ Reset Matrix...**
3. In the **Reset Matrix** dialog box enter,

Recharge Flux [L/T] = 0.00025 (this is the mean recharge rate of the two seasons)
Layer Indicator [IRCH]= 0
Recharge Options: Recharge is applied to the highest active cell

4. Click **OK** to exit the dialog box.
5. Leave the **Data Editor** by **File ▸ Leave Editor ▸ Yes**

Specified Flux Boundary

As MODFLOW does not have a separate package for specified flux boundary condition, we use the Well package to simulate this boundary condition.

▸ **To specify the boundary flux**

1. Select **Models ▸ MODFLOW ▸ Well**
2. Make sure the cell selected is [1,36,1]. Since the width of this cell is 500 m, the inflow rate throuth this cell is 500 m × 0.0672 m^3/day/m = 33.6 m^3/day. Click the right mouse button to open the **Cell Value** dialog box and enter 33.6 then click **OK** to exit the dialog box. A positive value means that water enters the system.
3. Specify the value 33.6 to the cell [2,36,1], the value 16.8 to the cells [3, 36 ,1] and [4, 36, 1] and the value 11.2 to the rest of the South boundary..
4. Leave the **Data Editor** by **File ▸ Leave Editor ▸ Yes**

Step 5: Perform steady-state flow simulation

You are just about ready to run the flow model. Quickly review the data that you have entered for each of the parameters and checking the values of various cells. Correct any data that do not look right, by redoing the appropriate section above. When checking any data entered under the **Models** menu item choose **Edit** rather than **Deactivate**.

▸ **To run the flow simulation**

1. Select **Models ▸ MODFLOW ▸ Run...**
2. Click **OK** to accept the warning regarding the Effective Porosity in the **Processing Modflow** dialog box.
3. Click **OK** in the **Run Modflow** dialog box to generate the required data files and to run MODFLOW, you will see a DOS window open and MODFLOW perform the iterations required to complete the flow simulation.
4. Press any key to exit the DOS Window.

Step 6: Extract and view results from the steady-state flow simulation

It is now time to view the results of your efforts, but first it is necessary to understand how the **Results Extractor** operates.

On occasions it is necessary to view some of the various sorts of output such as hydraulic heads and cell-by-cell flows generated by a MODFLOW simulation. This 2D data is accessed using the Results Extractor and saved in ASCII format on the computer's hard drive for use in other parts of PMWIN or in other programs such as SURFER or a spreadsheet program. It is quite a simple procedure to load and save any of the output generated by MODFLOW and in fact is a necessary first step in producing any form of graphical output from your MODFLOW simulations. The data files saved in the **Results Extractor** can be read back into the model using the **Data Editor**, this procedure will be explained shortly.

▸ **To load the head distribution after the steady state simulation**

1. Select **Tools ▸ Results Extractor…**
   You will see the **Results Extractor** dialog box which looks a little like a spreadsheet type window. In the **Results Type** box at the top of the dialog box it is possible to choose the sort of data you wish to load, while the **Stress Period, Time Step** and **Layer** boxes allow you to select the layer and time of the results loaded. If you choose the other tabs (MOC3D, MT3D, MT3DMS), you are presented with another choice as to which set of concentration terms you would like to load. At the moment however we are only concerned with the hydraulic head distribution.
2. Make sure Hydraulic Head is selected in the **Results Type** box.
3. Click the mouse button on **Read**, the hydraulic head values for the steady state solution will appear in the spreadsheet.
4. We will need to view this data graphically and to use it as the starting heads for the transient simulation so choose **Save…**
5. In the **Save Matrix As** dialog box enter T1SS.DAT as the filename and click on **OK** to exit the dialog box.
6. Click on **Close** to exit the **Results Extractor** dialog box.

As mentioned above it is possible to save any form of output generated by MODFLOW as a 2D ASCII data file for use in PMWIN or other software. The **Data Editor** is used to load a particular data file as input data for the MODFLOW simulation, all that needs to be done is start the **Data Editor** for the parameter you wish to modify. Data files may be created in other software packages and imported as long as the format is the same as that required by PMWIN.

The general procedure for loading data files into the model will be demonstrated using the head values since we need to visualise these and also use them as the starting heads in the following transient simulation.

Step 7: Produce output from the steady-state flow simulation

Visualization and output is best performed in the Presentation part of the program as this will not affect any part of the MODFLOW data.

▸ **To load the data into the Presentation matrix**

1. From the main menu select **Tools ▸ Presentation**
2. Open the **Browse Matrix** dialog box by **Value ▸ Matrix...**
3. In the **Browse Matrix** dialog box select **Load** to open the **Load Matrix** dialog box.
4. Click on  and select the appropriate file to load. In this case it is T1SS.DAT. Now click on OK.
5. Exit the **Load Matrix** dialog box by clicking on **OK**.
   The data will appear in the **Browse Matrix** dialog box, click on **OK** to exit this dialog box and return to the **Data Editor**. The data is now loaded.

▸ **To view contours of the data**

1. Select **Options ▸ Environment**... to open the **Environment Options** dialog box.
2. Click the **Contours** tab and make sure the **Visible** box is checked. Click on the header **Level** of the table to change the contour minumum to 12.5, maximum to 19 and the contour interval to 0.5. It is also possible to change contour color if you desire. If **Fill Contours** is checked, the contours will be filled with the colors given in the **Fill** column of the table. Use the **Label Format** button to specify an appropriate format.
3. Click **OK** to exit the **Environment Options** dialog box. Contours should now appear and if everything has gone well they will look similar to Fig. 6.4. Note the display of the model grid is deactived by using the **Environment Options** dialog box.
4. You may use **File ▸ Save Plot As…** or **File ▸ Print Plot...** to save or print the plot.
5. Leave the **Presentation** by **File ▸ Leave Editor ▸ Yes**

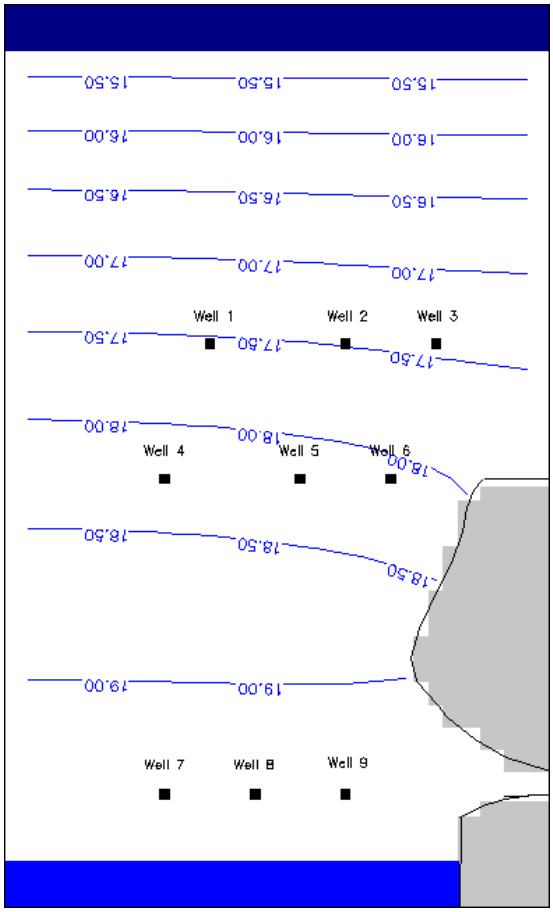


Fig. 6.4 Steady-state head distribution

Step 8: Transient Flow Simulation

Initial Hydraulic Head

It is now time to perform the transient simulations with the wet season recharge (120 days) and dry season pumping (240 days). The hydraulic heads resulting from the steady state simulation are used as the starting heads for the transient analysis.

- ▸ **To set the steady state heads as the starting values for the simulation**

1. Select **Parameters** ▸ **Initial Hydraulic Heads**
2. Open the **Browse Matrix** dialog box by **Value** ▸ **Matrix...**
3. In the **Browse Matrix** dialog box select **Load** to open the **Load Matrix** dialog box.
4. Click on  to open the **Load Matrix** dialog box and select the appropriate file to load, in this case it is T1SS.DAT. Click **OK**.

5. Exit the **Load Matrix** dialog box by clicking on **OK**.
6. The data will appear in the **Browse Matrix** dialog box, click on **OK** to exit this dialog box. The data is now loaded.
7. Leave the **Data Editor** by **File ▸ Leave Editor ▸ Yes**

Time Parameters

We now need to change from a steady state simulation to a transient simulation. In the transient simulation there are two stress periods, one of 240 days when pumping is occurring and no recharge and the other of 120 days when there is recharge only. It is possible to have different conditions for each stress period as will be demonstrated below.

▸ **To change to a transient simulation**

1. Select **Parameters ▸ Time...** to open the **Time Parameters** dialog box.
2. Change the model to transient by clicking on **Transient** in the Simulation Flow Type box.
3. Activate the second period by checking the **Active** box in the second row of the table.
4. Change the period length and time steps such that
   For period 1: Period Length = 240; Time Step = 12
   For period 2: Period Length = 120; Time Step = 6
5. Click **OK** to exit the **Time Parameters** dialog box.

Pumping rates

Now we need to set the pumping rate for each well during stress period 1.

▸ **To set the pumping rate**

1. Select **Models ▸ MODFLOW ▸ Well**
2. At each of the wells (marked by a little shaded box on the DXF Map) click the left mouse button to select the cell and then the right mouse button to set the pumping rate to -3888 in the **Cell Value** dialog box. This pumping rate is equivalent to 45 l/s, the negative sign means that water is being extracted from the system. A recharge well would have a positive sign.
3. Exit the **Data Editor** by **File ▸ Leave Editor**
   Upon leaving you are presented with a **Temporal Data** dialog box, this allows you to select and edit the data so that different values can apply during different Stress Periods.
4. Select Period 2 and click on **Edit Data**. The status bar displays Period 2 indicating that you are entering data for stress period 2.
5. For each well in the system set the pumping rate to 0 (this is the default value).

6. Exit the **Data Editor** by **File ▸ Leave Editor**, which again brings up the **Temporal Data** dialog box.
7. Exit the **Temporal Data** dialog box and the **Data Editor** by **Leave Editor ▸ Yes**

Recharge rates

There are two recharge periods, namely the dry season when recharge is zero and the wet season when recharge is 7.5×10^{-4} m/day.

▸ **To specify the recharge rate**

1. Select **Models ▸ MODFLOW ▸ Recharge ▸ Edit**
2. Set the entire grid to a uniform value for the first Stress Period by **Value ▸ Reset Matrix...**
3. In the **Reset Matrix** dialog box enter,
   Recharge Flux [L/T] = 0.0
   Layer Indicator [IRCH]= 0
   Recharge Options: Recharge is applied to the highest active cell
4. Click **OK** to exit the dialog box.
5. Leave the Data Editor by **File ▸ Leave Editor**, which brings up the **Temporal Data** dialog box.
6. Select Period 2 and click on **Edit Data** to edit the data for that period.
7. Using the above procedure change the recharge flux for the entire grid to 0.00075 (the values for the layer indicator and recharge option remain the same).
8. Exit the **Data Editor** by **File ▸ Leave Editor**, which again brings up the **Temporal Data** dialog box.
9. Exit the **Temporal Data** dialog box and the **Data Editor** by **Leave Editor ▸ Yes**

Specific Yield

Before running the transient simulation it is necessary to set the aquifer specific yield to 0.06.

▸ **To specify the specific yield**

1. Select **Parameters ▸ Specific Yield**
2. Set the entire grid to 0.06 and exit the **Data Editor** by **File ▸ Leave Editor ▸ Yes**

Run transient flow simulation

▸ **To run the flow simulation**

1. Select **Models ▸ MODFLOW ▸ Run...**
2. Click OK to accept the warning regarding the Effective Porosity in the **Processing Modlflow** dialog box.
3. Click OK in the **Run Modflow** dialog box to generate the required data files and to run MODFLOW, you will see a DOS window open and MODFLOW perform the iterations required to complete the flow simulation.
4. Press any key to exit the DOS Window.

Produce output

Using the **Presentation** tool and the **Results Extractor**, you can create contour plots for the water level at the end of each time step. The water level at the end of the pumping period (dry season) corresponds to the heads in time step 12 of period 1 (Fig. 6.5). The water level at the end of the recharge period (wet season) corresponds to the heads in time step 6 of period 2 (Fig. 6.6). Both figures use the contour interval of 0.5m. The minumum and maximum contour levels are 12.5m and 19m respectively.

Animation

Now, we can create an animation sequence to show the development of the water level during the wet and dry seasons.

▸ **To create an animation sequence**

1. Before creating an animation sequence, open the **Enivironment Option** dialog box to make sure that the contours are set to visible and the contour levels are set properly.
2. Select **File ▸ Animation...**
3. In the **Animation** dialog box, click the **open file** button  .
   A **Save File** dialog box appears. Select or specify a base filename for the animation files in the dialog box, then click **Open**. Note that you cannot save the animation files in the same folder as your model data. So, you need first to create a new folder or select another folder for the files.
4. Check **Create New Frames**, set **Result Type** to Hydraulic Head and set **Display Time (s)** to 0.2. Like a movie, an animation sequence is based on lots of frames. Each frame is saved by using the filenames *fn.xxx*, where *fn* is the **Frame File** specified above and *xxx* is the serial number of the frame files. **Display Time** is the display duration for each frame.
5. In the **Animation** dialog box, click **OK** to start the animation.

PMWIN will create a frame (image) for each time point at which the simulation results (here: hydraulic head) are saved. When all frames are created, PMWIN will repeat the animation indefinitely until the **Esc** key is pressed.

Once a sequence is created, you can playback the animation at a later time by repeating the above steps with **Create New Frames** cleared. You can also use the **Animator** (provided by PMWIN) to playback the sequence.

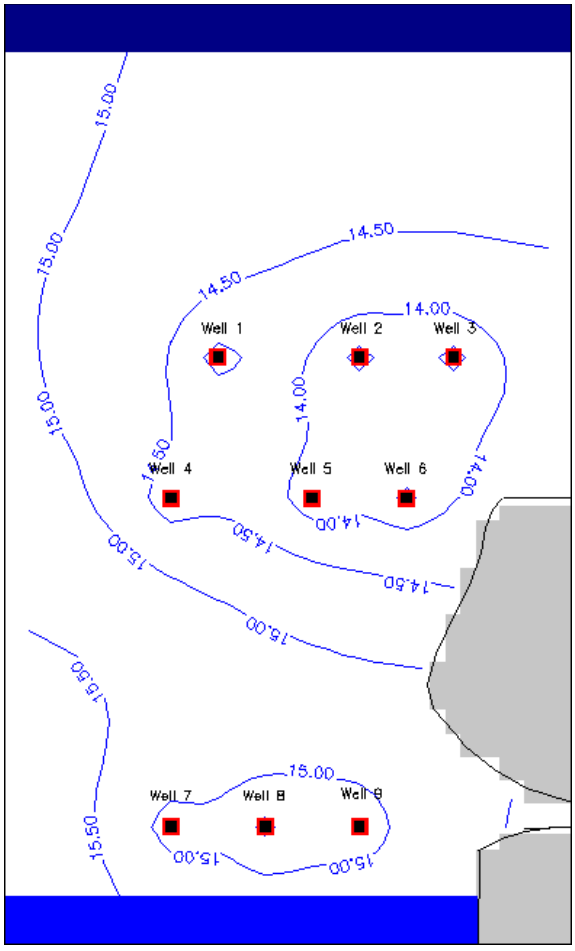


Fig 6.5 Head distribution after 240 days of pumping (period 1, time step 12)

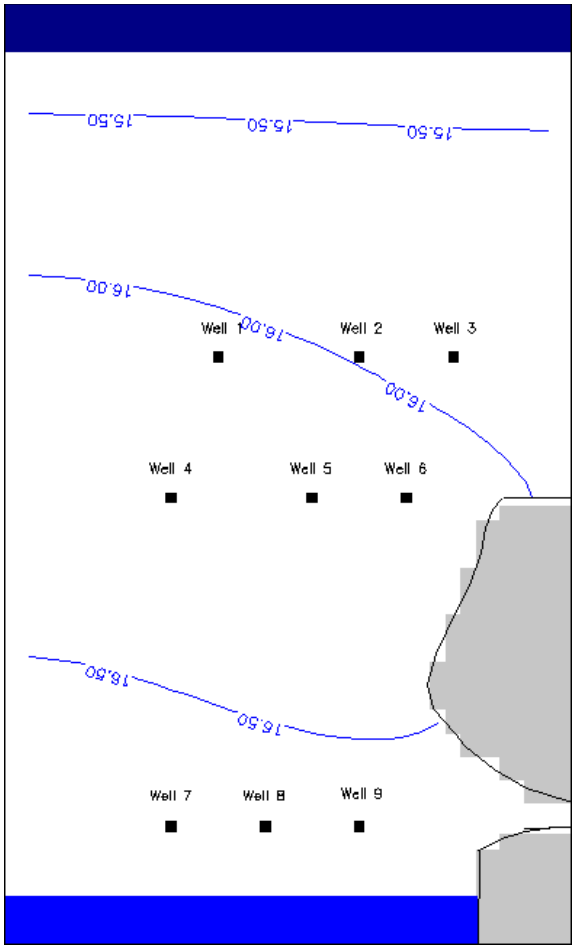


Fig. 6.6 Head distribution after 120 days of recharge (period 2, time step 6)

6.1.2 Tutorial 2 - Confined and Unconfined Aquifer System with River

Folder: \pm5\examples\tutorials\tutorial2\

Overview of the Problem

A river flows through a valley (Fig. 6.7) which is bounded to the north and south by impermeable granitic intrusions. The hydraulic heads at the upstream and downstream fixed-head boundaries are known (which are saved in a data file). The river forms part of a permeable unconfined aquifer system (horizontal hydraulic conductivity K_h = 5 m/day, vertical hydraulic conductivity K_v = 0.5 m/day, specific yield Sy = 0.05, effective porosity n_e= 0.2) which overlies a confined aquifer of a variable thickness (K_h = 2 m/day, K_v= 1 m/day, specific storage Ss = 5×10^{-5}, n_e = 0.25). A 2 m thick silty layer (K_h = 0.5 m/day, K_v = 0.05 m/day, n_e = 0.25) separates the two aquifers. The elevations of the aquifer tops and bottoms are known (and saved in data files). Three pumping wells pumping at 500 m^3/day each abstract water from the confined aquifer.

Your task is to construct a 3 layer groundwater flow model of the area including the river and the pumping wells and to assess the capture zone of the wells.

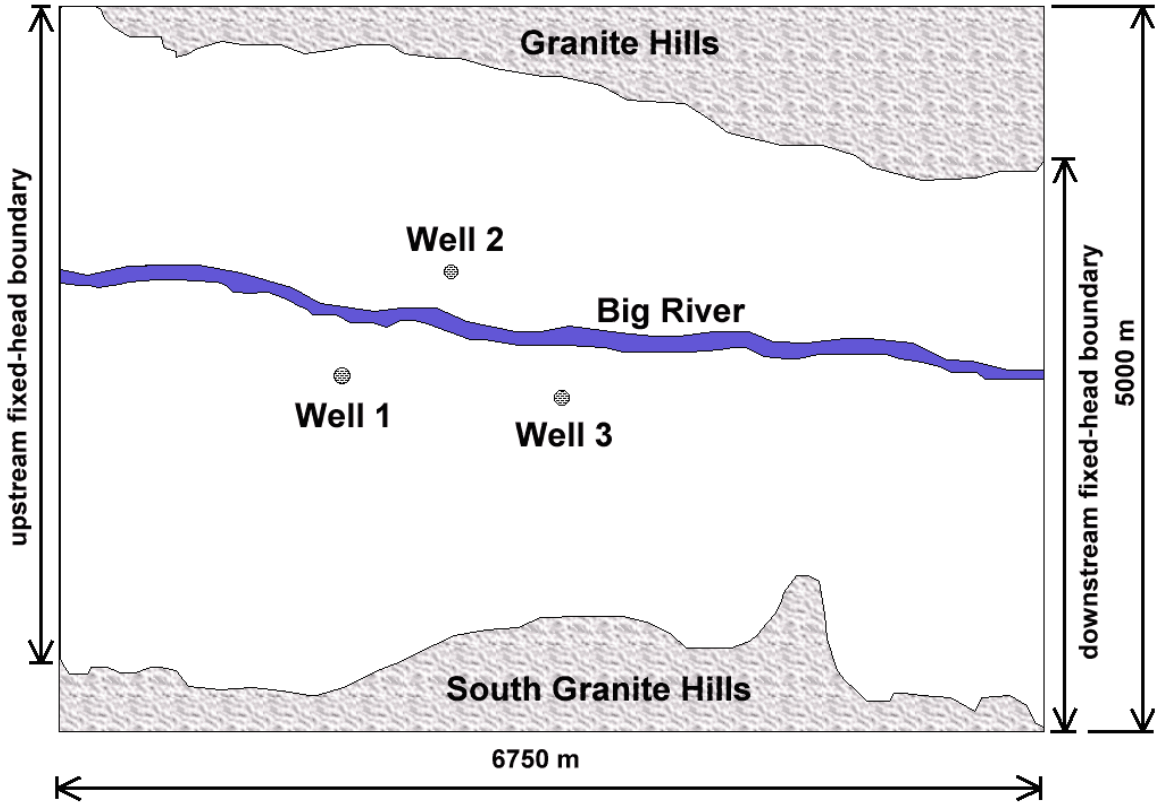


Fig. 6.7 Model area

Step 1: Create a New Model

▸ **To create a new model**

1. Select **File ▸ New Model...**
2. In the New Model dialog box, change the working folder to \pm5\examples\T2 (create the folder, if it does not exist) and enter T2 as the name of the new model.
3. Click **OK** to exit the dialog box.

Step 2: Define Model Size

▸ **To define the size of the model**

1. Select **Grid ▸ Mesh Size...**
2. In the **Model Dimension** dialog box enter,

Layers	Number	3
Columns	Number	27
	Size	250
Rows	Number	20
	Size	250

3. Click **OK** to exit this dialog box.

You are now in the **Grid Editor** of the PMWIN. To help visualize the problem we can overlay a DXF file as a map, which gives us the locations of the boundaries and the pumping wells.

▸ **To load a map**

1. Select **Options ▸ Maps…** to open the **Map Options** dialog box.
2. Click the box beside the space for the DXF filename to activate that particular map (it is also possible to choose a color by clicking on the colored square.
3. In the first filename field of DXF-files, click the right mouse button to bring up the **Map Files** dialog box.
4. Choose BASEMAP2.DXF from the folder \pm5\examples\tutorials\tutorial2\, click **OK** to exit the dialog box.

5 Click **OK** to exit the **Map Options** dialog box.
You will see that it does not match the grid that you have generated.

▸ **To move the grid**

1. Select **Options ▸ Environment...** to open the **Environment Options** dialog box.
2. Enter X_0= 200 and Y_0=6000 and click **OK** to exit the dialog box.

3. Leave the **Data Editor** by **File ▸ Leave Editor ▸ Yes**

Step 3: Refine Model Grid

▸ **To refine the model grid**

1. Select **Grid ▸ Mesh Size**.
2. Refine the mesh around each of the three wells by halving the size of the following rows and columns:
   Columns 8, 9, 10, 11, 12, 13 and 14
   Rows 7, 8, 9, 10, 11 and 12
   The grid should now be refined around the wells and appear similar to Fig. 6.8.
3. Leave the **Data Editor** by **File ▸ Leave Editor ▸ Yes**

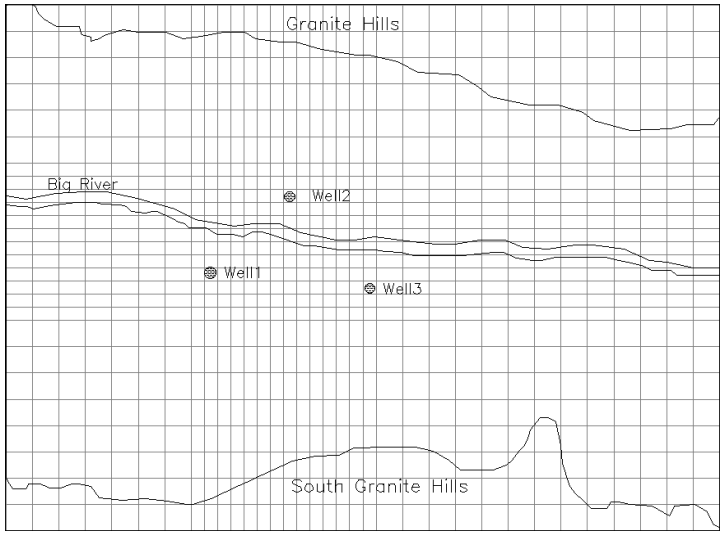


Fig. 6.8 Model discretization

Step 4: Assign Model Data

All the following data will be entered using the **Data Editor**. The unconfined aquifer is the layer 1 in the model. The silty layer and the confined aquifer is simply layer 2 and layer 3, it is possible to switch between layers in the **Data Editor** by using the **Page Up** and **Page Down** keys on the keyboard.

Aquifer types

▸ **To define the aquifer types**

1. Open the **Layer Options** dialog box by **Grid ▸ Layer Type...**

2. Make sure that for layer 1 the type is set to **1:unconfined** and that Layers 2 and 3 are set to **3:confined/unconfined**.
3. Click **OK** to exit the **Layer Options** dialog box.

Flow boundaries

▸ **To specify the IBOUND data**

1. Select **Grid ▸ Boundary Condition ▸ IBOUND (Modflow)**
2. Set fixed-head boundaries (IBOUND = -1) in layer 1 and layer 3 (use  to switch Layer Copy on or off and use the Page Up and Page Down keys to switch between layers) at the west and east boundaries where the river enters and leaves the model area. Note that the horizontal flow component in the second layer (silty layer) is negligible, so we do not need to specify fixed-head cells in this layer.
3. Set no-flow boundaries in all layers in the areas defined by the Granite and South Granite Hills. The boundaries in layers 1 and 3 should look like those in Fig. 6.9. The boundaries in the layer 2 should look like those in Fig. 6.10.
4. Leave the **Data Editor** by **File ▸ Leave Editor ▸ Yes**

Aquifer geometry

The top of each aquifer slopes gradually from west to east. To save you entering this data, the top elevation of each aquifer has been saved as a data file.

▸ **To specify the top elevation of each aquifer**

1. Select **Grid ▸ Top of Layers (TOP).**
2. Import the file \pm5\examples\tutorials\tutorial2\aq1top.dat as the elevation of the top of aquifer 1 using **Value ▸ Matrix ▸ Load...** etc.
3. Switch to Layer 2 by pressing the **Page Down** (PgDn) key.
4. Import the file \pm5\examples\tutorials\tutorial2\aq2top.dat as the elevation of the top of aquifer 2.
5. Switch to Layer 3 by pressing the **Page Down** (PgDn) key.
6. Import the file \pm5\examples\tutorials\tutorial2\aq3top.dat as the elevation of the top of aquifer 2.
7. Leave the **Data Editor** by **File ▸ Leave Editor ▸ Yes**

▸ **To specify the bottom elevation of each aquifer**

1. Select **Grid ▸ Bottom of Layers (BOT).**
   PMWIN will ask if you want to use the Top of Layer 2 as the Bottom of Layer 1, and Top of Layer 3 as the Bottom of Layer 2. We will accept this. Note that the elevation of the bottom of the layer 3 is 0.0 m, so we do not need to change the default value.
2. Leave the **Data Editor** by **File ▸ Leave Editor ▸ Yes**

Specification of the geometry of the system is now complete, all we need to do now is enter the physical parameters of the system.

Fig. 6.9 Boundary Conditions in layer 1 and layer 3

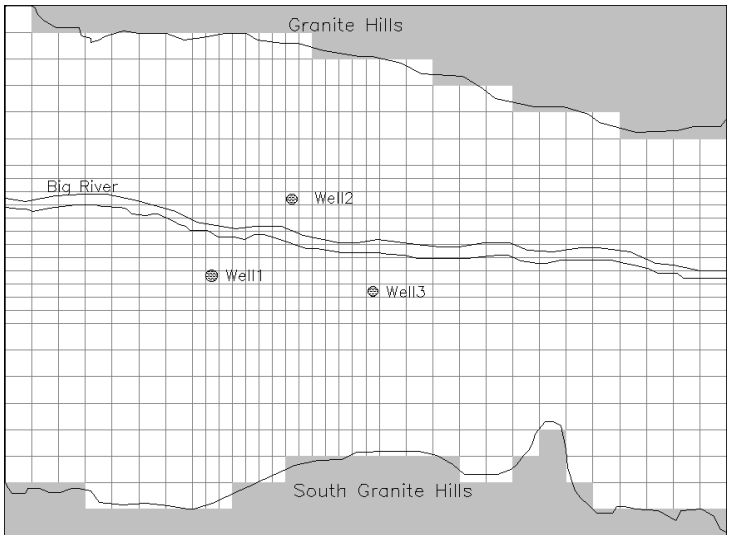


Fig. 6.10 Boundary Conditions in layer 2

Time parameters

▸ **To specify the time parameters**

1. Select **Parameters ▸ Time**...
2. In the **Time Parameters** dialog box, change the Simulation Time Unit to **DAYS** and check the **Steady-State** is selected in the Simulation Flow Type box.
3. Click OK to leave the **Time Parameters** dialog box.

Initial hydraulic heads

The groundwater flows naturally under a gentle gradient towards the river from both sets of hills and also in an easterly direction. The values of starting heads (which include the required values for the fixed-head cells) are saved in the file \pm5\examples\tutorials\tutorial1\t2sh.dat.

▸ **To load the initial hydraulic heads**

1. Select **Parameters ▸ Initial Hydraulic Heads**
2. Open the **Browse Matrix** dialog box by **Value ▸ Matrix...**
3. In the **Browse Matrix** dialog box select **Load** to open the **Load Matrix** dialog box.
4. Click on  and select the file \pm5\examples\tutorials\tutorial1\t2sh.dat to load. Now click on OK.
5. Exit the **Load Matrix** dialog box by clicking on **OK**.
   The data will appear in the **Browse Matrix** dialog box, click on **OK** to exit this dialog box and return to the **Data Editor**. The data is now loaded into layer 1.
6. Turn on **layer copy** by pressing down the **layer copy** button.
7. Move to the second layer and the third layer by pressing PgDn twice. Now, the data of layer 1 is copied to the second and third layers.
8. Leave the **Data Editor** by **File ▸ Leave Editor ▸ Yes**

Hydraulic Conductivity

▸ **To set the horizontal hydraulic conductivity**

1. Select **Parameters ▸ Horizontal Hydraulic Conductivity**
2. Use **Value ▸ Reset Matrix...** to enter the following data,

   Layer 1 5.0 m/day
   Layer 2 0.5 m/day
   Layer 3 2.0 m/day

3. Leave the **Data Editor** by **File ▸ Leave Editor ▸ Yes**

▸ **To set the vertical hydraulic conductivity**

1. Select **Parameters ▸ Vertical Hydraulic Conductivity**
2. Use **Value ▸ Reset Matrix...** to enter the following data for each layer
   Layer 1 0.5 m/day
   Layer 2 0.05 m/day
   Layer 3 1.0 m/day
3. Leave the **Data Editor** by **File ▸ Leave Editor ▸ Yes**

Effective Porosity

The effective porosity is used in PMPATH, which we will use later to define the capture zones of the pumping wells.

▸ **To specify the effective porosity**

1. Select **Parameters ▸ Effective Porosity**
2. Use **Value ▸ Reset Matrix...** to enter the following data for each layer
   Layer 1 0.2
   Layer 2 0.25
   Layer 3 0.25
3. Leave the **Data Editor** by **File ▸ Leave Editor ▸ Yes**

River

The River data is a little difficult to set up. MODFLOW requires that the river stage (ie. head), river bottom elevation, and riverbed conductance be specified. The riverbed conductance is defined as:

$$CRIV = \frac{K \cdot L \cdot W}{M}$$

where,

CRIV = hydraulic conductance of the riverbed [L^2/T]
K = hydraulic conductivity of the riverbed sediment [L/T]
L = length of the river within a cell [L]
W = width of the river within a cell [L]
M = thickness of the riverbed [L]

In our case the riverbed has the following properties:

K = 2 m/day
L = 250 or 125 m depending on the length of the river within the cell
W = 100 m
M = 1 m

▸ **To specify the river data**

1. Select **Models ▸ MODFLOW ▸ River**
2. You will notice that the river meanders across the model domain and rarely is contained within a single cell. First, you need to decide the river data for each cell using the equation above. The river data is entered by selecting the appropriate cell with the left mouse button and then clicking with the right mouse button to enter the river data associated with that cell. Entering the river data is sometimes very cumbersome. Fortunately, we have saved the *river hydraulic conductance*, *head* and *elevation of the riverbed bottom* in three ASCII matrix files, so we need only to import them.
3. To import river data, select **Value ▸ Matrix...**. In the **Browse Matrix** dialog box, select *River Hydraulic Conductance* from the **Parameter** drop-down box, then click **Load...** to import the conductance file \pm5\examples\tutorials\tutorial2\t2riverc.dat. Select *Head in the River* from the **Parameter** drop-down box, then click **Load...** to import the head file \pm5\examples\tutorials\tutorial2\t2riverh.dat. Finally, select *Elevation of the Riverbed Bottom*, then click **Load...** to import the file \pm5\examples\tutorials\tutorial2\t2riverb.dat. You should see the cells specified as river cells highlighted in light blue.
4. Leave the **Data Editor** by **File ▸ Leave Editor ▸ Yes**

Wells

▸ **To specify the well data**

1. Select **Models ▸ MOFLOW ▸ Well**
2. Switch to Layer 3 by pressing the PgDn key twice.
3. Move the grid cursor to Well 1 by clicking on it with the left mouse button and set the pumping rate to -500 [m^3/day] by bringing up the **Cell Value** dialog box with the right mouse button.
4. Repeat the above step with Well 2 and Well 3.
5. Leave the **Data Editor** by **File ▸ Leave Editor ▸ Yes**

Step 5: Perform steady-state flow Simulation

▸ **To run the flow simulation**

1. Select **Models ▸ MODFLOW ▸ Run...**
2. Click **OK** in the **Run Modflow** dialog box to generate the required data files and to run MODFLOW, you will see a DOS window open and MODFLOW perform the iterations required to complete the flow simulation.
3. Press any key to exit the DOS Window.

Step 6: Extract and view results

▸ **To produce head contours**

1. Using the **Results Extractor**, save the hydraulic head data as T2S1.DAT and T2S2.DAT and T2S3.DAT for Layer 1, 2 and 3 respectively.
2. Select **Tools ▸ Presentation** and load the saved data into each layer. Alternatively, you may open the **Results Extractor** dialog box within the **Data Editor** by **Value ▸ Result Extractor**. In this case, the **Results Extractor** dialog box will contain an additional **Apply** button, which allows to put the data from the **Results Extractor** to the model grid directly.
3. Use **Options ▸ Environment...** to choose the settings of the contours. The contour plot for the first model layer should look similar to that in Fig 6.11.

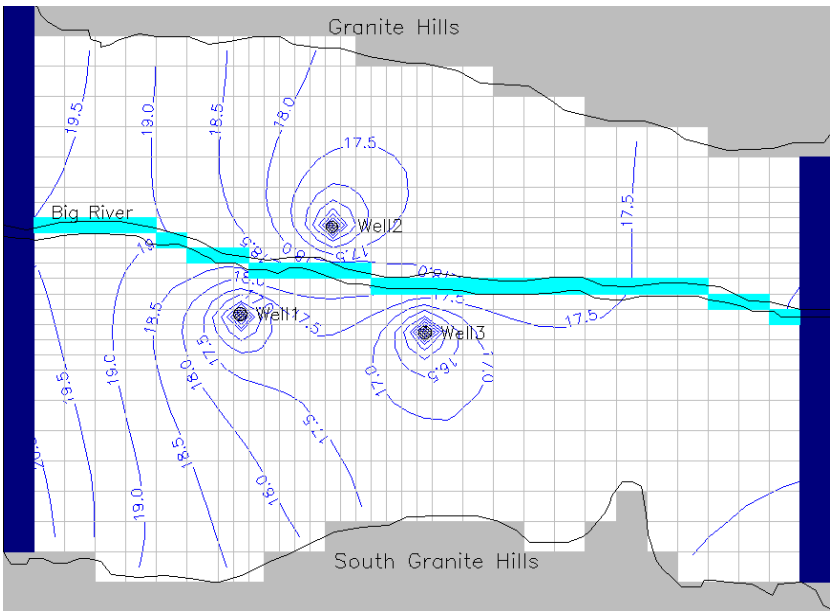


Fig. 6.11 Steady-state head distribution in the first model layer

▸ **To delineate the capture zones of the pumping wells**

1. Start PMPATH by **Models ▸ PMPATH (Pathlines and contours).**
   PMPATH will load the current model automatically. We will place particles around the pumping wells and examine their 10 year capture zones.
2. Move to Layer 3 by pressing the Page Down (PgDn) key twice.
3. Click on the + button and drag a small box around the cell containing Well 1 by holding down the left mouse button and moving the mouse.
4. When you release the mouse button the **Add New Particles** dialog box appears, edit **Particles on circles** such that the number of particles is equal to 15, the radius R = 80 and the number of planes NK=3.
5. Click the **Properties** tab and change the color of new particles to Blue.
6. Click on **OK** to exit the **Add New Particles** dialog box.
7. Using a similar procedure add particles around Well 2 and Well 3. Make each of these a different color (say Green and Black).
8. To display the hydraulic heads and a transverse and longitudinal cross section open the **Environment Options** dialog box by **Options ▸ Environment…**
9. Click the **Contours** tab, check the **Visible** box and click on the **Restore Defaults** button to get standard settings.
10. Click the **Cross Sections** tab, check the **Visible** and **Show grid** boxes and set Exaggeration=25, Projection Row=15 and Projection Column=9.
11. Click on **OK** to exit the **Environment Options** dialog box.
    The hydraulic head contours for layer 3 and cross sections showing the location of the particles should appear.
12. To set up the particle tracking parameters, open the **Particle Tracking (Time) Properties** dialog box by **Options ▸ Particle Tracking (Time).** In the **Tracking Steps** group, change the (time) unit to years, step length to 10 and maximum number of steps to 200.
13. Click OK to exit the **Particle Tracking (Time) Properties** dialog box.
14. Start the backward particle tracking by **Run ▸ Backward**.
    You can easily see that the flowlines intersect with the river in numerous places (Fig. 6.12).
15. You can produce a plot of the steady state hydraulic heads of Layer 3 and the flowlines by **File ▸ Save Plot As…**

▸ **To run forward particle tracking**

We will now introduce a contaminant source upstream of Well 2 and see how far the contamination moves through the steady state flow field after 75, 100 and 125 years.

1. Since the contamination is a surface source we need to place the particles in layer 1, if you

aren't already in Layer 1 change to it by using the Page Up (PgUp) key.

2. To place the particles on the ground surface, drag a box around the cell [6, 5, 1].
3. In the **Cell Faces** tab of the **Add New Particles** dialog box you will notice that the figure defines the various faces of an individual cell, since the contamination is a surface source we only want to place particles on cell face 5.
4. Click the **Particles** tab and set the number of particles on Face 5 to NI=4 and NJ=4 and set NI and NJ on all the other faces to 0.
5. Click **OK** to leave the **Add New Particles** dialog box.
6. Open the **Particle Tracking (Time) Properties** dialog box by **Options ▸ Particle Tracking (Time)...**
7. In the **Tracking Steps** group, change the (time) unit to years, step length to 1, and maximum number of steps to 75. When finished, click **OK** to leave the dialog box.
8. Start the backward particle tracking by **Run ▸ Forward**.
9. Repeat the above for Maximum number of steps of 100 and 125. The plot generated after 125 steps should look similar to Fig. 6.13.

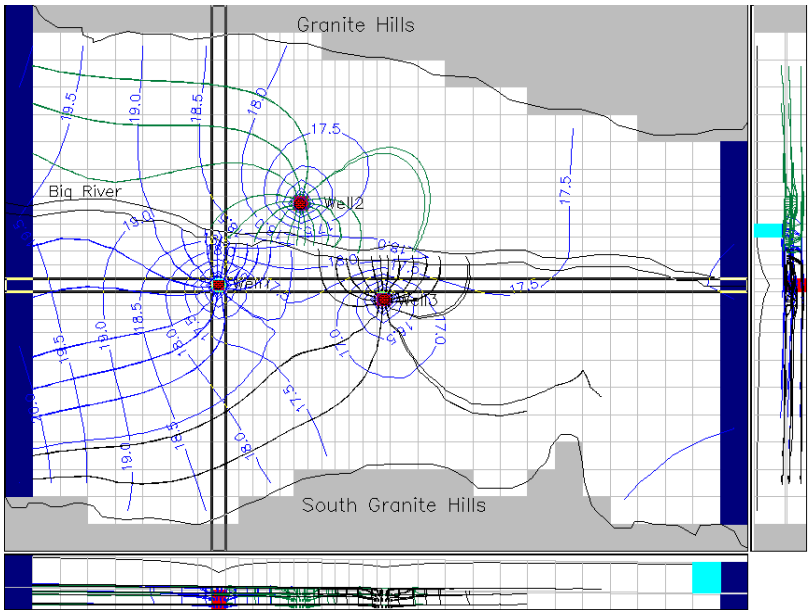


Fig. 6.12 Steady-state hydraulic head distribution in the third model layer and capture zones of pumping wells

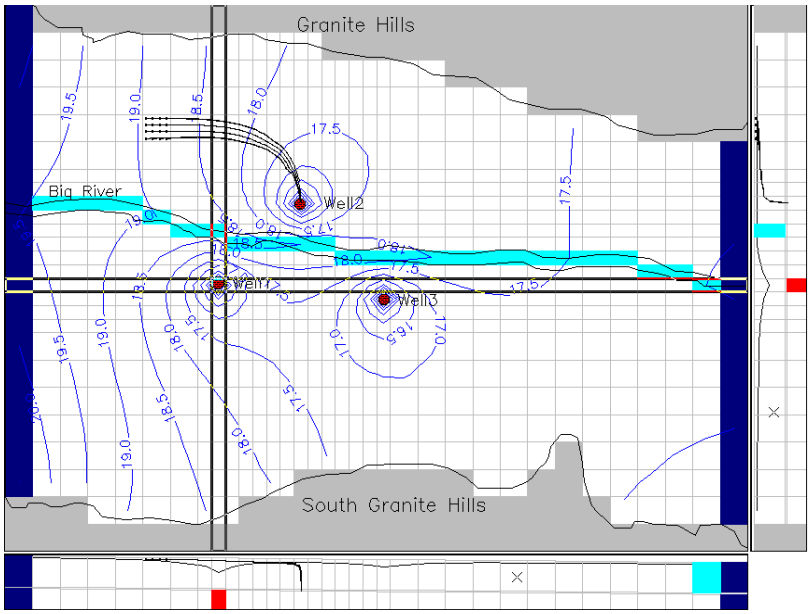


Fig. 6.13 125 years streamlines; particles are started at the cell [6, 5, 1] and flow towards Well 2

6.2 Basic Flow Problems

6.2.1 Determination of Catchment Areas

Folder: \pm5\examples\basic\basic1\

Overview of the Problem

Fig. 6.14 shows a part of an unconfined aquifer. The extent of the aquifer to the North and South is assumed to be unlimited. The aquifer is homogeneous and isotropic with a measured horizontal hydraulic conductivity of 0.0005 m/s and an effective porosity of 0.1. The elevations of the aquifer top and bottom are 15 m and 0 m, respectively. The aquifer is bounded by a no-flow zone to the west. To the east exists a river, which is in direct hydraulic connection with the aquifer and can be treated as fixed-head boundary. The river width is 50 m and stage is 10m. The mean groundwater recharge rate is 8×10^{-9} m/s. A pumping well is located at a distance of 1000 m from the river.

Your task is to calculate the catchment area of the well and the 365-days-capture zone under steady-state flow conditions.

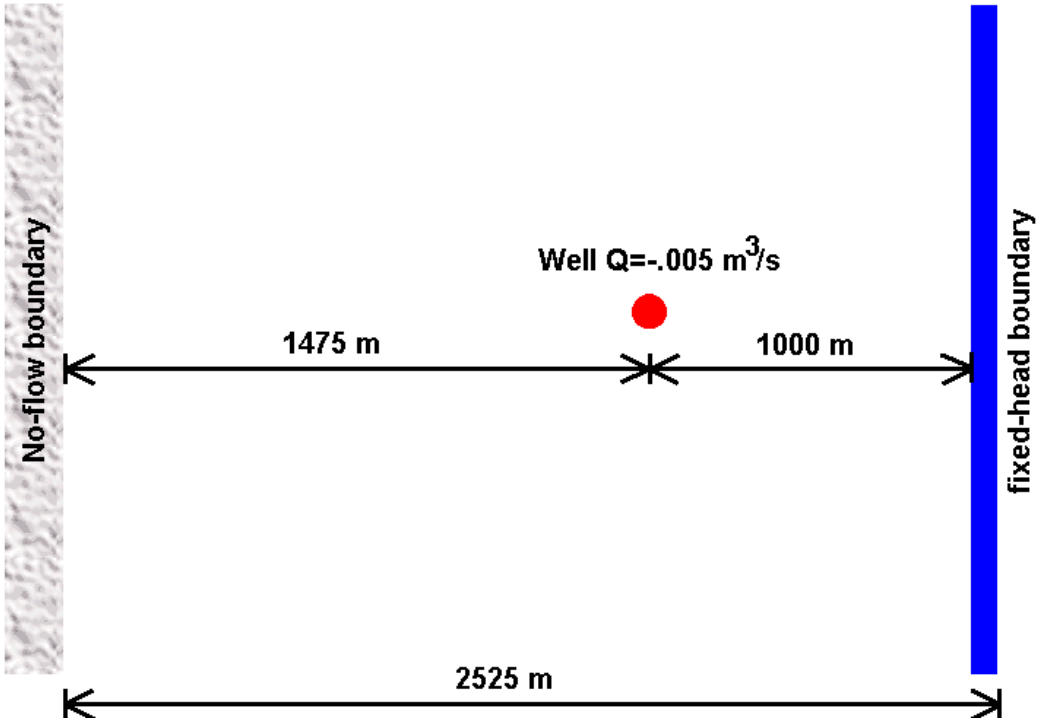


Fig. 6.14 Plan view of the model area

Modeling Approach and Simulation Results

The west boundary of the model is impervious and the river to the east is simulated by the fixed-head boundary condition (IBOUND=-1) with the initial head at 10 m. There are no natural boundaries to the South and North, so we have to use streamlines as impervious boundaries. The distance of the selected streamline from the well must be large enough, so that the hydraulic head at these boundaries are not affected by the pumping well. This is the case if the total recharge in the chosen strip is considerably larger than the pumping rate of the well. Because of the symmetry of the system, we could use one-half of the model area only. To show the whole catchment area, we decided to use the entire model area.

The aquifer is simulated using a grid of one layer, 50 rows and 51 columns. A regular grid space of 50 m is used for each column and row. The layer type is **1: unconfined**. Fig. 6.15 shows the contours, the catchment area and the 365-days-isochrones of the pumping well using a 2D-approach, where the groundwater recharge is treated as a distributed source within the model cells and 50 particles are initially placed around the pumping well in the middle of the aquifer. If the groundwater recharge is applied on the groundwater surface (refer to RCH/EVT options in chapter 4 for this option), particles will be tracked back to the groundwater surface (Fig. 6.16). We can easily imagine that the size and form of the calculated catchment area depend on the boundary condition, recharge rate and starting (vertical) position of particles and the vertical position of the well screen, if the well is only partially penetrating. A discussion about the determination of catchment areas in two and three spatial dimensions can be found in Kinzelbach et al. (1992).

To delineate the catchment area of a pumping well in a 3D flow field, we must place enough particles around and along the well screen. Fig. 6. 17 shows the catchment area calculated by PMPATH. First, 425 particles are placed around the well by using the **Add New Particles** dialog box (the settings are NI=5, NJ=5 on faces 5 and 6 and 25 particles on the circles with R=25 and NK=15 around the pumping well). Then backward tracking is applied for a duration of 100 years. Finally, the end points of the particles are saved by **File ▸ Save Particles As...**. This file can be reloaded into PMPATH by **File ▸ Load Particles** to display the catchment area.

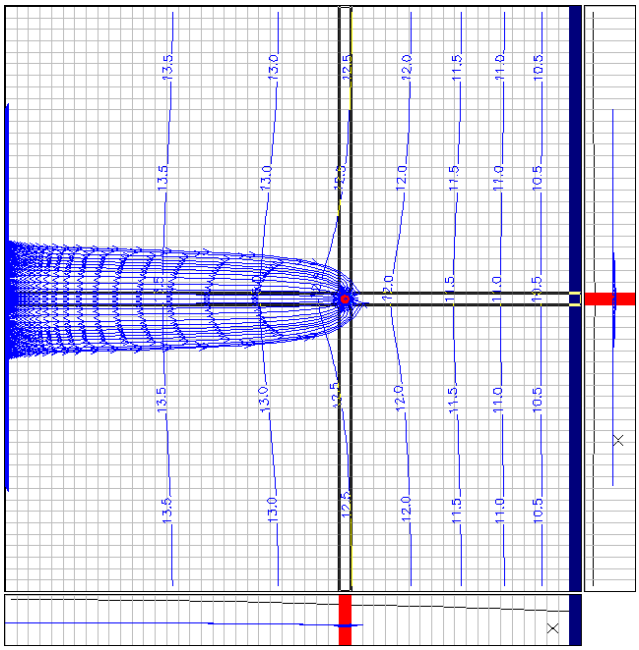


Fig. 6.15 Catchment area and 365-days isochrones of the pumping well (2D-approach: groundwater recharge is treated as distributed source within the model cells).

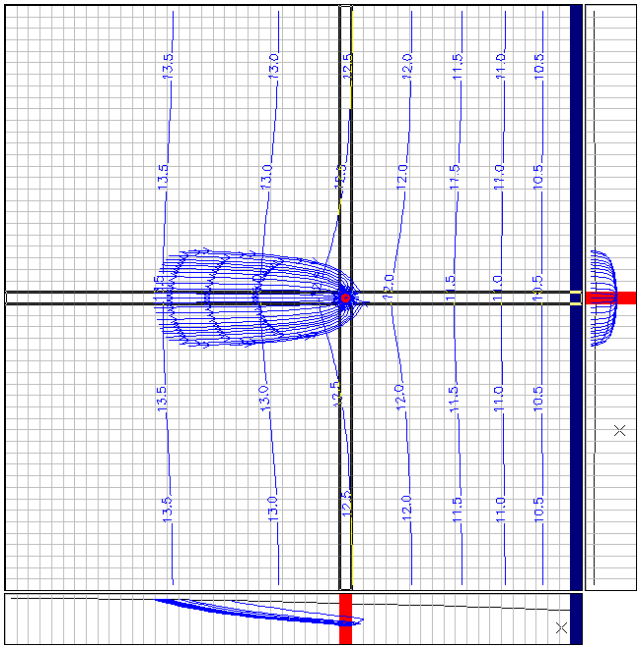


Fig. 6.16 Particles are tracked back to the groundwater surface by applying the groundwater recharge on the groundwater surface.

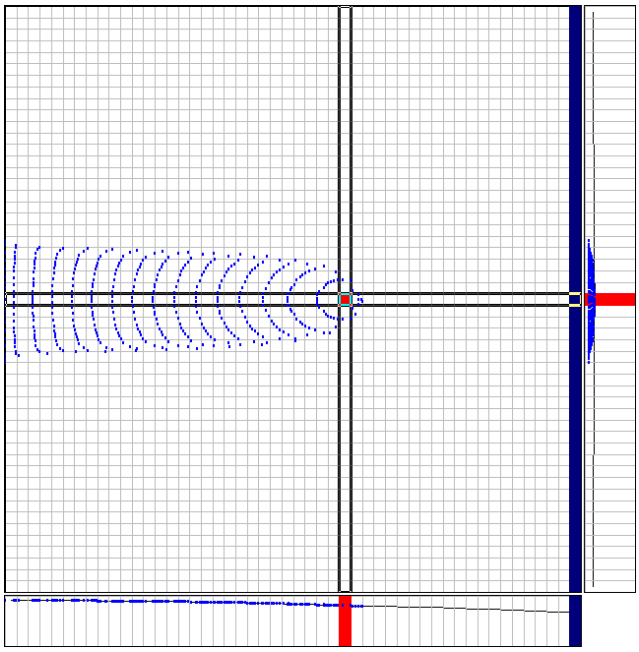


Fig. 6.17 Catchment area of the pumping well (3D-approach).

6.2.2 Use of the General-Head Boundary Condition

Folder: \pm5\examples\basic\basic2\

Overview of the Problem

This simple example demonstrates the use of the general-head boundary package of MODFLOW. A confined, homogeneous and isotropic aquifer is shown in Fig. 6.18. The aquifer is bounded by a no-flow zones to the north and south. The hydraulic heads at the west and east boundaries are 12m and 10m, respectively. The transmissivity of the aquifer is T = 0.01 m^2/s. The aquifer has a constant thickness of 10 m.

Your task is to calculate the head contours for the case that only the west part of the aquifer is modelled. The east boundary of the modelled part should be approached by using the general-head boundary.

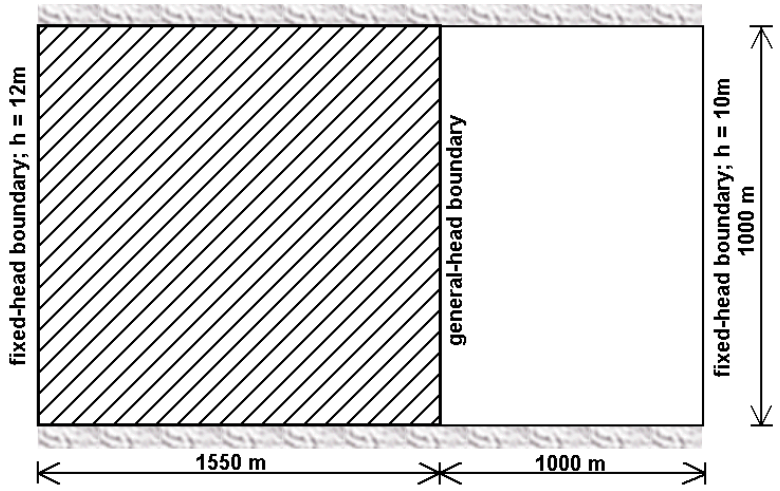


Fig. 6.18 Plan view of the model area

Modeling Approach and simulation results

The aquifer is simulated using a grid containing 1 layer, 10 rows and 16 columns. A regular grid spacing of 100 m is used for each column and row. The layer type is **0: confined** and the **Transmissivity** flag in the **Layer Options** dialog box is **User-specified**. The initial hydraulic head is 12 m everywhere. While the west model boundary is simulated by the fixed-head boundary condition (IBOUND=-1) with the initial head at 12 m, the east boundary is simulated by the general-head boundary (GHB) condition with the head h = 10 m. Analogous to the

riverbed hydraulic conductance (eq. 3.21), the hydraulic conductance term of each GHB cell is $C_b = K \cdot A / L$, where K is the (horizontal) hydraulic conductivity, L is the distance from the actual fixed-head boundary to the modelled GHB cell, and A is the area of the cell face, which is perpendicular to the groundwater flow in the un-modelled area. For this example $C_b = (T/10) \cdot (100 \cdot 10) / 1000 = 0.001$ m^2/s.

Fig. 6.19 shows the calculated contours. For comparison, the entire aquifer is modelled with the east and west fixed-head boundaries and the result is shown in Fig. 6.20. The model is saved in the folder \pm5\examples\basic\basic2a\.

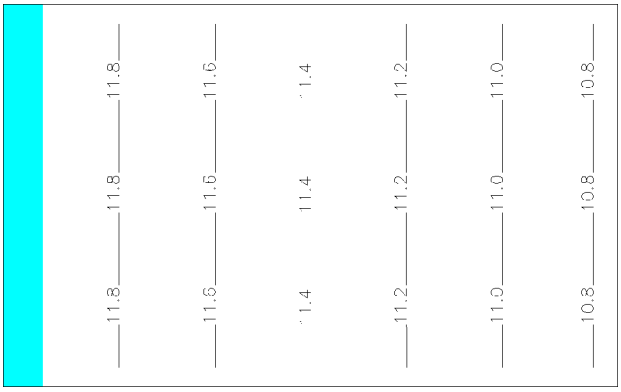


Fig. 6.19 Calculated head contours for the west part of the aquifer

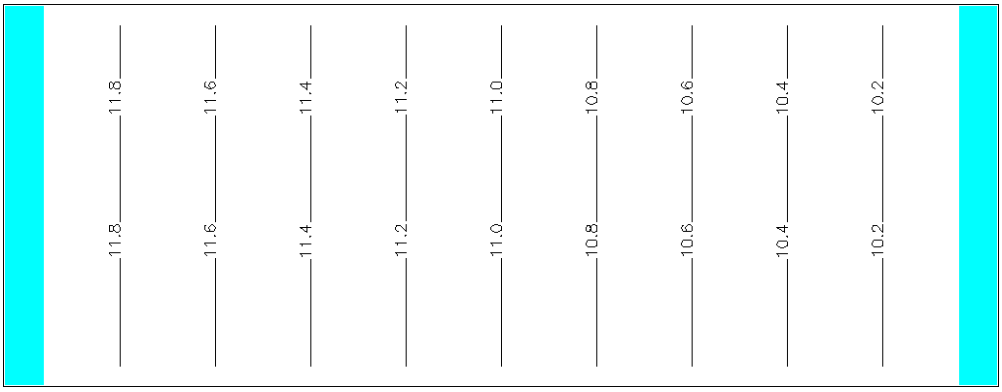


Fig. 6.20 Calculated head contours for the entire aquifer

6.2.3 Simulation of a Two-Layer Aquifer System in which the Top Layer Converts between Wet and Dry

Folder: \pm5\examples\basic\basic3\

Overview of the Problem

This example is the first test problem of the BCF2 package (McDonald et al., 1991). In an aquifer system where two aquifers are separated by a confining bed, large pumpage withdrawals from the bottom aquifer can desaturate parts of the upper aquifer. If pumpage is discontinued, resaturation of the upper aquifer can occur.

Fig. 6.21 shows two aquifers separated by a confining unit. No-flow boundaries surround the system on all sides, except that the lower aquifer discharges to a stream along the right side of the area. Recharge from precipitation is applied evenly over the entire area. The stream penetrates the lower aquifer; in the region above the stream, the upper aquifer and confining unit are missing. Under natural conditions, recharge flows through the system to the stream. Under stressed conditions, two wells withdraw water from the lower aquifer. If enough water is pumped, cells in the upper aquifer will desaturate. Removal of the stresses will then cause the desaturated areas to resaturate.

Your task is to construct a model to compute the natural steady-state head distribution, and then calculate the head distribution under the stressed condition. When solving for natural conditions, the top aquifer initially is specified as being entirely dry and many cells must convert to wet. When solving for pumping condition, the top aquifer is initially specified to be under natural conditions and many cells must convert to dry.

Modeling Approach and Simulation Results

The model consists of two layers - one for each aquifer. Because horizontal flow in the confining bed is small compared to horizontal flow in the aquifers and storage is not a factor in steady-state simulations, the confining bed is not treated as a separate model layer. The effect of the confining bed is incorporated in the value for vertical leakance (see section Fig. 3.15). Note that if storage in the confining bed were significant, transient simulations would require that the confining layer be simulated using one or more layers. The confining layer must also be simulated, if you intend to calculate pathlines with PMPATH or to simulate solute transport. A uniform horizontal grid of 10 rows and 15 columns is used. Aquifer parameters are specified as shown in Fig. 6.21.

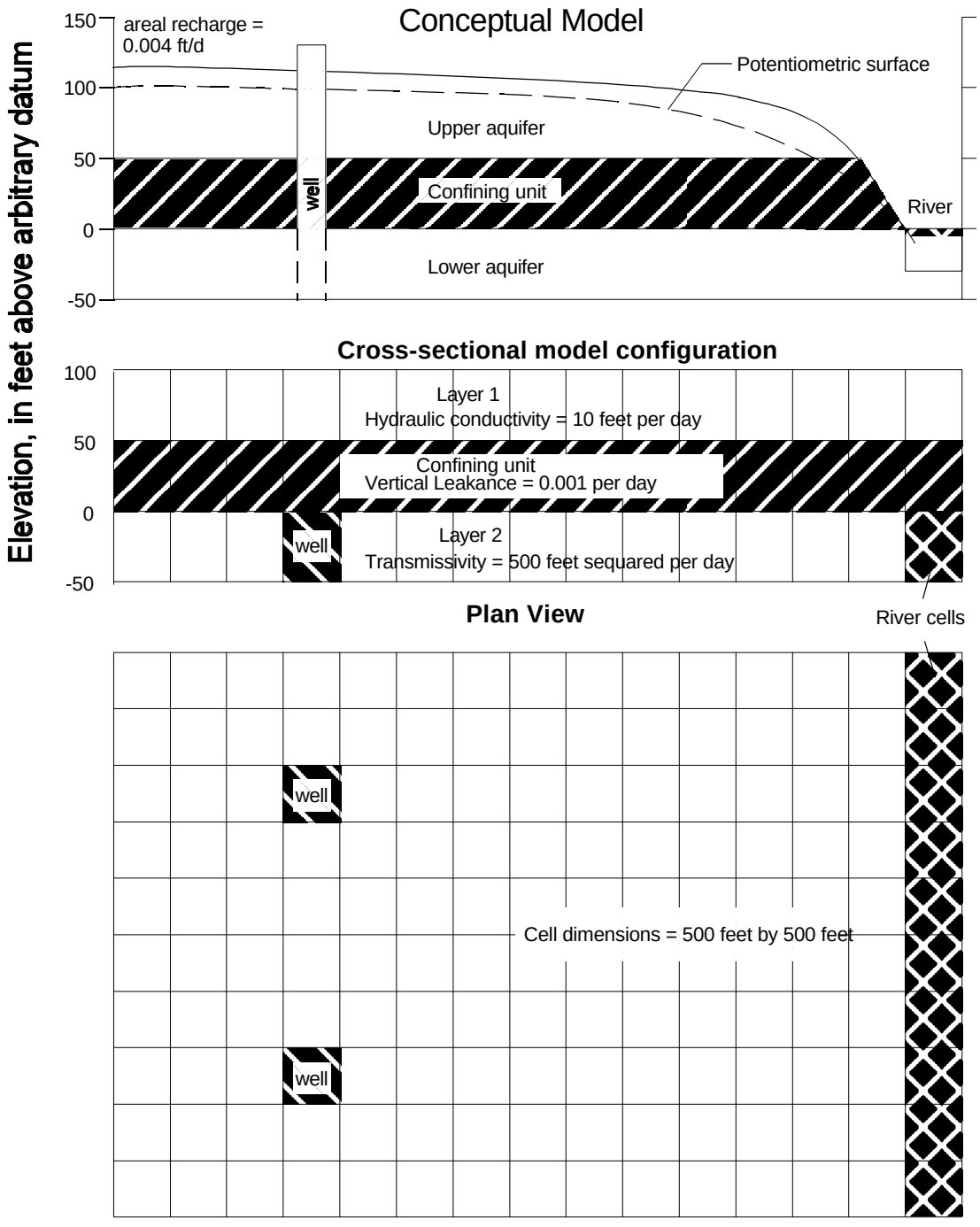


Fig. 6.21 Configuration of the hypothetical model (after McDonald et al., 1991).

Two steady-state solutions were obtained to simulate natural conditions and pumping conditions. The steady-state solutions were obtained through a single simulation consisting of two stress periods. The first stress period simulates natural conditions and the second period simulates the addition of pumping wells with extraction rates of 30000 ft^3/d (≈ 850 m^3/d). The simulation is declared to be steady state, so no storage values are specified and each stress period requires only a single time step to produce a steady-state result. The PCG2 Package is used to solve the flow equations for the simulations.

Determination of the wetting threshold THRESH (see **Modflow ▸ Wetting Capability...**) often requires considerable effort. The user may have to make multiple test runs trying different values in different areas of the model. In many cases, positive THRESH values may lead to numerical instability and therefore the user should try negative THRESH values first.

6.2.4 Simulation of a Water-Table Mound resulting from Local Recharge

Folder: \pm5\examples\basic\basic4\

Overview of the Problem

This example is the second test problem of the BCF2 package. Localized recharge to a water-table aquifer results in formation of a ground-water mound. For example, a ground-water mound may form in response to recharge from infiltration ponds commonly used to artificially replenish aquifers or to remove contamination by filtration through a soil column. If the aquifer has low vertical hydraulic conductivity or contains interspersed zones of low hydraulic conductivity, it may be necessary to simulate the aquifer using multiple model layers in which the mound crosses more than one layer.

The conceptual model consists of a rectangular, unconfined aquifer overlain by a thick unsaturated zone (Fig. 6.22). The horizontal hydraulic conductivity is 5 feet per day and vertical hydraulic conductivity is 0.25 feet per day (≈ 0.0762 m/d). A leaking pond recharges the aquifer, resulting in the formation of a ground-water mound. The pond covers approximately 6 acres (≈ 23225 m^2) and pond leakage is 12,500 cubic feet per day (≈ 354 m^3/d). The specific yield is 20 percent. The water table is flat prior to the creation of the recharge pond. The flat water table is the result of a uniform fixed-head boundary that surrounds the aquifer.

Your task is to calculate the water table under the steady-state condition and the formation of the groundwater mound over time.

Modeling Approach and Simulation Results

Because of the symmetry, heads are identical in each quadrant of the aquifer, and there is no flow between quadrants; therefore, only one quarter of the system needs to be simulated. The problem is simulated using a grid of 40 rows, 40 columns, and 14 layers (Fig. 6.22). A uniform horizontal grid spacing of 125 feet (≈38.1 m) is used, and each layer is 5 feet (≈1.52 m) thick. The pond is in the upper left corner of the grid. The boundaries along row 1 and column 1 are no-flow as a result of the symmetry. A fixed-head boundary of 25 feet (≈7.62 m) is specified along row 40 and column 40 for layers 10-14; a no-flow boundary is assigned along row 40 and column 40 for layers 1-9. Without the recharge from the pond, layers 1-9 are dry, and the head in all the cells of layers 10-14 is 25 feet. Recharge from the pond is applied to the horizontal area encompassed by rows 1 through 2 and columns 1 through 2. Recharge option *"Recharge is applied to the highest active cell"* is used so that recharge will penetrate through inactive cells down to the

water table. The specific recharge rate of 0.05 foot per day (≈0.0152 m/d) simulates leakage of 3,125 cubic feet per day (≈88.5m^3/d) through one quarter of the pond bottom, a simulated area of 62,500 square feet (≈5806 m^2).

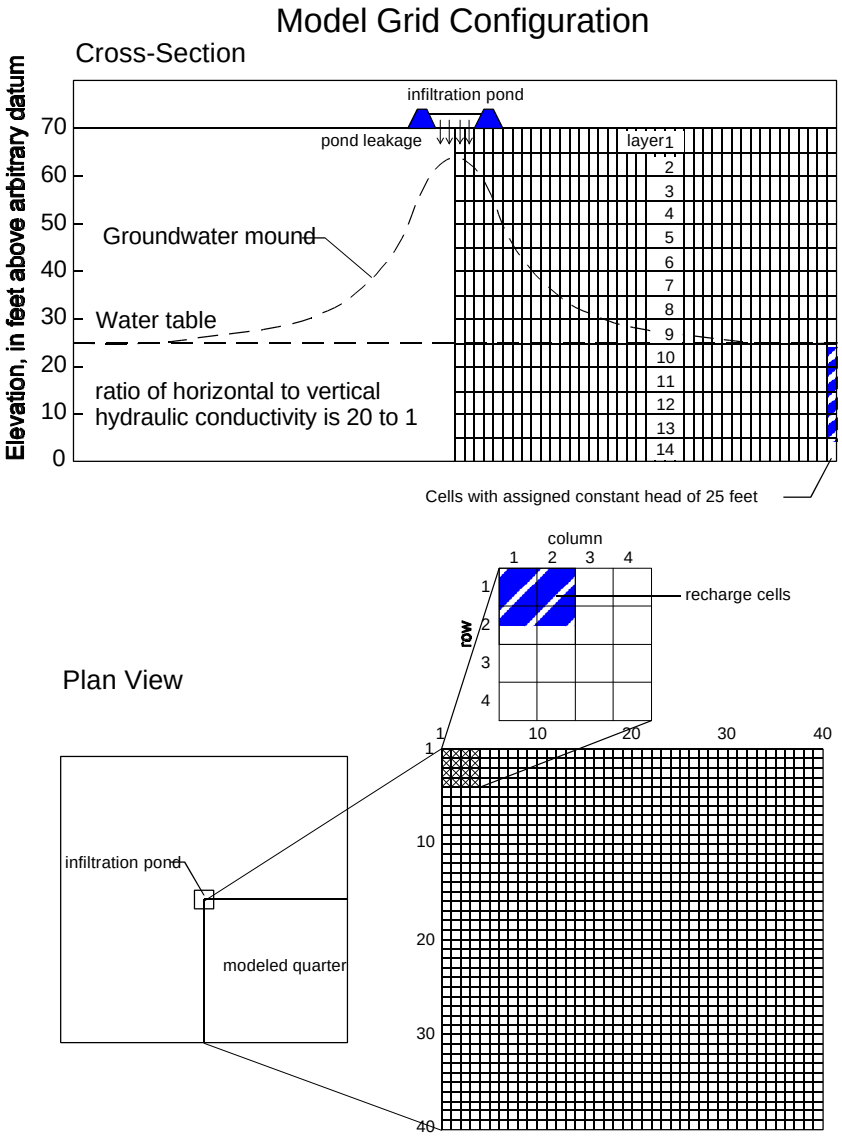


Fig. 6.22 Hydrogeology and model grid configuration

Reasonable solutions to the ground-water mounding problem can be obtained in two steady-state simulations by using the PCG2 solver. In the first simulation, dry cells are converted to wet by comparison of the wetting threshold THRESH to heads in underlying cells only, which is

indicated by a negative value of THRESH. The wetting-iteration interval is 1 and THRESH is -0.5 foot, which means that the wetting threshold is 10 percent of the thickness of a cell. In the second simulation, wetting of cells is based on comparison to heads both in horizontally adjacent and underlying cells (THRESH is positive). A wetting-iteration interval of 2 and a THRESH of 1.5 feet are used in order to prevent continued oscillation between wet and dry for some cells. Due to the steepness of the head gradient and the grid discretization, the head difference between adjacent horizontal cells is generally much larger than the head difference between adjacent vertical cells along the mound. For example, the cell at layer 4, row 3, column 4 is supposed to be dry even though the head in the horizontally adjacent cell in column 3 is 1.4 feet above the bottom of the layer. The vertical head difference between cells in this part of the model is much less; the difference between the head at the cell in layer 4, row 3, column 3 and the cell below is only 0.05 foot. Thus, the neighboring cell to the right is repeatedly and incorrectly converted to wet during the solution process if horizontal wetting is used with a wetting threshold of 0.5 foot. The larger wetting threshold and wetting-iteration interval used in the second simulation allow convergence to occur, but only after many iterations. In this simulation, head in adjacent vertical cells is the best indicator of when a dry cell should become wet.

The formation of the groundwater mound over time can be obtained with a transient simulation. The transient simulation is run for one stress period with a length of 500,000 days. The stress period is divided into 50 time steps with a time-step multiplier of 1.3. The first time step is 0.3 days, and the last time step is 115,385 days. The specific yield is 20 percent and the confined storage coefficient is 0.001. The PCG2 solver is used and cells are activated by comparison of the wetting threshold to heads in underlying cells. The head change criterion for closure is 0.001 foot and the residual-change criterion is 10,000 cubic feet, the wetting threshold is 0.5 foot, the wetting factor is 0.5, and the wetting-iteration interval is 1. Fig. 6.23 shows simulated water-table heads along row 1 at several times during the transient simulation. Steady-state conditions were reached at the 44th time step of the transient simulation as indicated by storage flow terms being zero (see the simulation listing file OUTPUT.DAT).

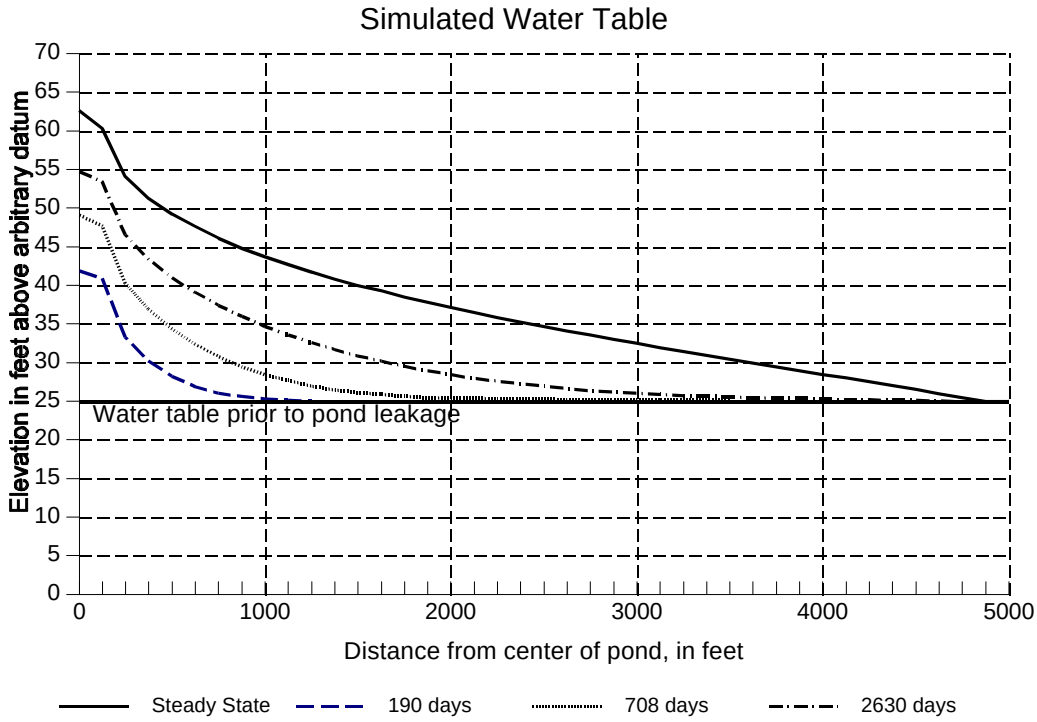


Fig. 6.23 Simulated water-table heads along row 1 beneath a leaking pond after 190 days, 708 days, 2630 days and steady state conditions (after McDonald et al., 1991)

6.2.5 Simulation of a Perched Water Table

Folder: \pm5\examples\basic\basic5\

Overview of the Problem

This example is the third test problem of the BCF2 Package. Contrasts in vertical hydraulic conductivity within the unsaturated zone can provide a mechanism for the formation of perched ground-water tables. The conceptual model is rectangular and consists of three geohydrologic units. The upper and lower units have higher hydraulic conductivities than the middle unit (Fig. 6.24). There is a regional water table in which the head is below the bottom of the middle unit. Natural recharge occurs over the entire area at a rate of 0.001 foot per day. This recharge can percolate through the two upper units without the formation of a water table above the middle because the vertical hydraulic conductivity of this unit is 0.002 foot per day.

Recharge at a rate of 0.01 foot per day from a pond covering 6 acres ($\approx$23225 m^2) will cause a perched ground-water body to form in the top two units. The total pond leakage is about 2,360 cubic feet per day ($\approx$66.8 m^3/d). The perched water table spreads out over an area much larger than the area covered by the pond. This has an impact on the distribution of recharge to the lower unit.

Your task is to calculate the long-term head distribution resulting from the pond recharge.

Modeling Approach and Simulation Results

Because of the rectangular symmetry of the system, there is no flow between quadrants. Therefore, only one quarter of the system must be simulated. The problem is simulated using a grid of 50 rows, 50 columns, and 2 model layers. A uniform grid spacing of 16 feet is used. The recharge pond is in the upper left corner of the grid; the quarter of the pond that is simulated occupies a square area that is 16 rows long and 16 columns wide. The boundaries along row 1 and along column 1 are no-flow boundaries as a result of the symmetry.

Model layer 1 simulates the upper geohydrologic unit and is assigned a hydraulic conductivity of 5 feet per day. The bottom of layer 1 is at an elevation of 20 feet. The lower geohydrologic unit is simulated as model layer 2. This layer is simulated as a confined/unconfined layer with constant transmissivity (layer type 2). The top and bottom elevations of layer 2 are set at 10 and 0 feet, respectively. Because the head in this layer is always below the layer top, the flow from above is limited as described by McDonald and Harbaugh (1988, p. 5-19). Thus, there is no direct hydraulic connection between the perched layer and the lower layer,

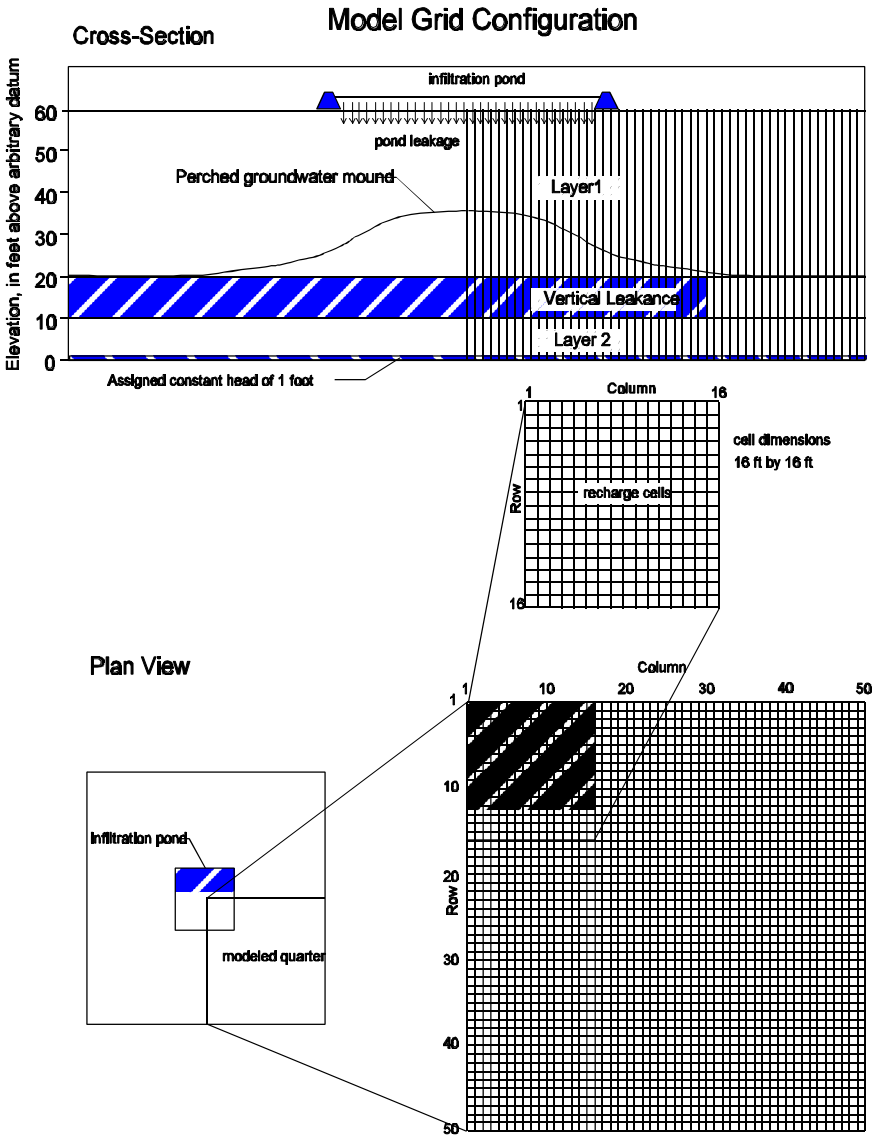


Fig. 6.24 Hydrogeology and model grid configuration

but the perched heads have a direct impact on the recharge into the lower layer. All cells in layer 2 are assigned a constant head of 1 foot because there is no need to simulate heads in this layer for the purpose of estimating recharge. The middle geohydrologic unit is not simulated as a separate model layer because it is assumed that horizontal flow and storage effects are negligible. This unit is represented by the value for vertical leakance between model layers 1 and 2. The vertical leakance is assumed to be 0.0002 per day. In areas not covered by the pond, recharge is applied areally at a rate of 0.001 foot per day to simulate natural recharge. Recharge option *"Recharge is applied to the highest active cell"* is used so that recharge will penetrate through

inactive cells to the water table. A recharge rate of 0.01 foot per day is applied to the area covered by the pond.

A steady-state simulation is performed to simulate the formation of a perched water table. Solution of the flow equation is obtained using the SIP solver. Starting hydraulic head in layer 1 under the pond is set at 21 feet. All other cells in layer 1 initially are specified as no-flow cells. The wetting-iteration interval, THRESH, and wetting factor are set at 2 iterations, 1.0 foot, and 0.5 foot, respectively (see **MODFLOW ▸ Wetting Capability**). A positive value of THRESH indicates that horizontally adjacent cells can cause dry cells to become wet. This is the only way for cells in layer 1 to become wet because heads in layer 2 are always below the bottom of layer 1.

Fig. 6.25 shows the contours of steady-state heads in layer 1. Steady-state heads along row 1 in layer 1 range from 29.92 feet in the cell [1, 1, 1] to 20.84 feet in cell [40, 1, 1].

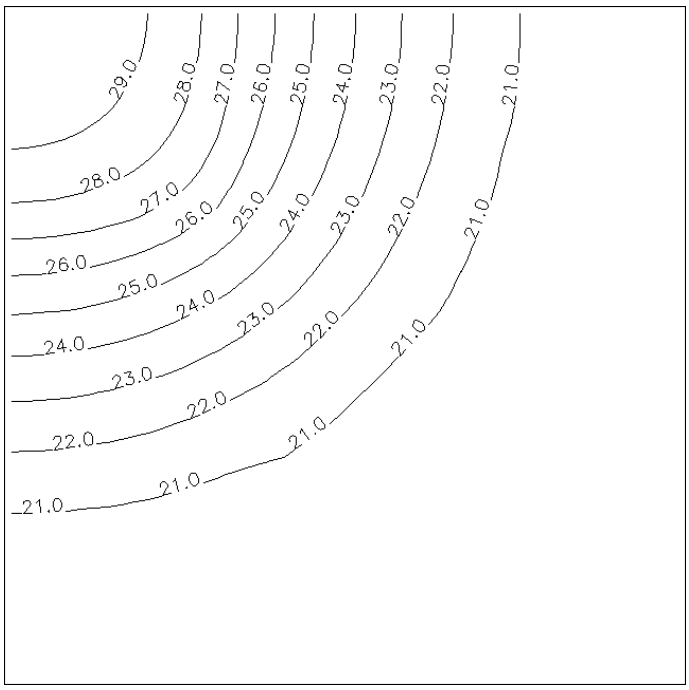


Fig. 6.25 Simulated steady-state head distribution in layer 1

6.2.6 Simulation of an Aquifer System with Irregular Recharge and a Stream

Folder: \pm5\examples\basic\basic6\

Overview of the Problem

This example is the first test problem of the Streamflow-Routing (STR1) package. Results from the STR1 Package were compared to results from an analytical solution developed by Oakes and Wilkinson (1972). An idealized aquifer with a river flowing through the middle was chosen and is shown in Fig. 6.26. The width of the aquifer perpendicular to the river was 4,000 ft on each side, while the length parallel to the river was 13,000 ft. Assumptions used in both the analytical solution and the model simulation include:

1. The lateral boundaries of the aquifer are impermeable (no flow is allowed).
2. The rocks beneath the aquifer are impermeable.
3. The river penetrates the entire depth of the aquifer and has vertical banks.
4. The river is not separated from the aquifer by any confining material.
5. The transmissivity and storage coefficient are constant throughout the aquifer and remain constant in time.
6. The aquifer is confined and Darcy's Law is valid.
7. The flow of groundwater is horizontal.
8. The water level in the river is constant along its length and with time.
9. The infiltration of recharge to the aquifer is instantaneous (no delay between the time precipitation infiltrates the surface until it reaches the water table).
10. The discharge from the aquifer is only to the river.

Transmissivity of the aquifer used for both the analytical solution and in the model simulation was 3,200 ft^2/d (3.45×10^{-3} m^2/s). The storage coefficient is 0.20. Because the river is assumed to be fully penetrating and the aquifer is not separated from the river by any confining material, the streambed conductance value was assumed equal to the transmissivity of the aquifer (in this example, the width of the river is assumed equal to the depth of the aquifer) times the length of the river in each cell (1,000 ft) divided by an assumed l-foot thickness of the riverbed. Actually, any large streambed conductance value can be used as long as the head value in the model cell containing the river remains constant during the simulation. Varying the streambed conductance value shows that for this problem, streambed conductances greater than 10 ft^2/d produce nearly the same results. Annual recharge to the aquifer is 1.5 ft. However, the daily recharge rate varied according to a sinusoidal distribution for the first 180 days, while no recharge was allowed for

the following 180 days. The distribution of the recharge over time is shown in Fig. 6.27.

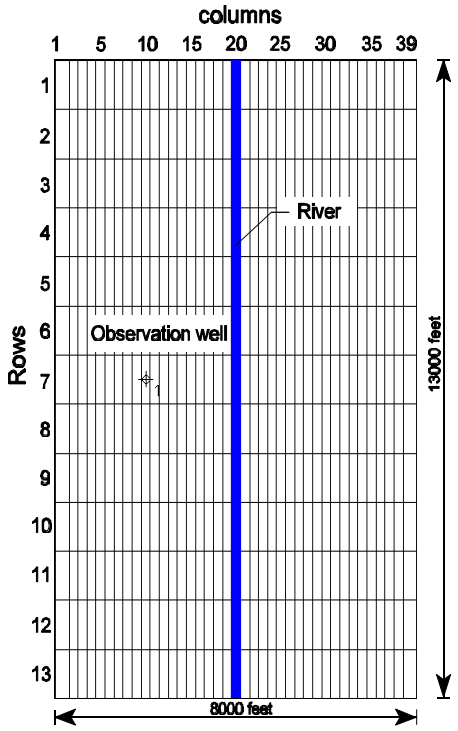


Fig. 6.26 Configuration of the model and the location of the observation well

Modeling Approach and Simulation Results

The aquifer is simulated using one model layer. Specification of the elevations of layer top and bottom are not necessary, because the layer is confined and transmissivity and confined storage coefficient are specified directly (as defined in the **Layer Options** dialog box). The sinusoidal distribution of the recharge rate was divided into 15-day intervals for the model simulation and the rate for the middle of each interval was used as input value. The distribution used in the simulation is also shown in Fig. 6.27. A total of six 360-day infiltration periods (144 stress periods, each with a length of 15 days) was used in the simulation. The first five 360-day infiltration periods were computed to allow the model to reach a stable yearly cycle because the starting water level for each model cell was not known. Results of the model simulation from the sixth infiltration period are compared to the results from the analytical solution for an observation well 2,000 ft from the river (Fig. 6.28). The coordinates of the observation well are given in the **Boreholes and Observations** dialog box. The Streamflow-Routing package is not really needed to simulate this condition, as the river could have been represented using fixed-head or river cells. The same results can be obtained using the River package. The simulation

was done to determine if the STR1 package correctly accumulates flow from the aquifer into the stream.

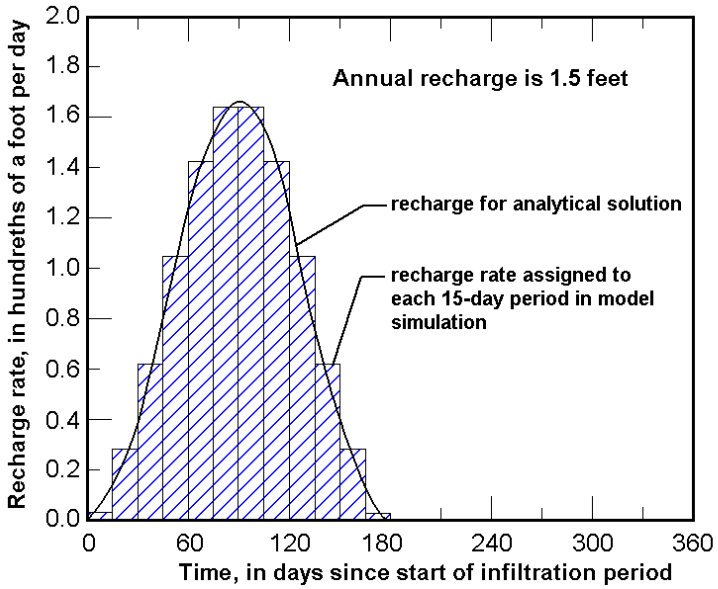


Fig. 6.27 Distribution of recharge used for analytical solution and the model simulation (after Prudic, 1988)

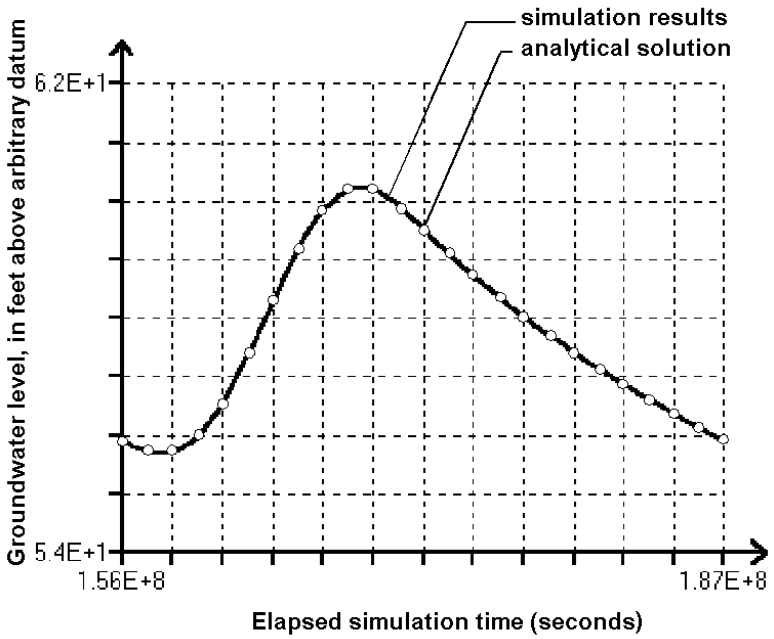


Fig. 6.28 Comparison of simulation results to analytical solution developed by Oakes and Wilkinson (1972)

6.2.7 Simulation of a Flood in a River

Folder: \pm5\examples\basic\basic7\

Overview of the Problem

This example is the second test problem of the STR1 package. The function of the STR1 package that computes the head in the stream as well as changes in flows to and from the aquifer was compared to an analytical solution developed by Cooper and Rorabaugh (1963). The model grid used in the previous example was also used in this model. The aquifer properties and assumptions are the same as those used in the previous example, except for assumptions 8 - 10, which are replaced with the following assumptions: (1) The recharge to the aquifer is only from the river as river stage increases with time and (2) The discharge from the aquifer is only to the river as river stage decreases with time.

The analytical solution from Cooper and Rorabaugh (1963, p. 355-358) is applicable for the case where the lateral boundary is at infinity (referred to by Cooper and Rorabaugh as semi-infinite). The impermeable boundary assigned at 4,000 ft for this model is of sufficient distance from the river in order not to interfere with the results. A flood in the river was simulated for a 30-day period.

The procedure used to calculate the distribution of streamflow for the 30-day period and for 60 days following the flood was first to calculate a distribution of river stage using equation 71 in Cooper and Rorabaugh (1963, p. 355), assuming a maximum flood stage of 4 ft above the initial river stage. The streamflow distribution (Fig. 6.29) was calculated from the river stage distribution. The river has a width of 100 ft, a dimensionless roughness coefficient of 0.02377 and a slope of 0.0001. A constant C = 1.486 should be used for the simulation (see eq. 3.22).

Modeling Approach and Simulation Results

Streamflow for the first 30 days was divided into l-day periods for simulation. Fig. 6.30 shows the computed river stage. The simulation results are the same as the manually calculated river stage values using equation 71 of Cooper and Rorabaugh (1963, p. 355). Detailed discussion on the analytical and numerical results can be found in Prudic (1988). Results of varying both the number of columns and the length of stress periods used to simulate the flood wave indicate that both the number of columns and the length of the time step are important in exactly duplicating the analytical solution.

A groundwater flow model with the Streamflow-Routing package has an advantage over

analytical solutions because it can be used to simulate complex systems. An example (**Folder:** \pm5\examples\basic\basic7a\) containing a stream system (Fig. 6.31) is used to illustrate most of the features of the Streamflow-Routing package. The example assumes that an aquifer of 6,000 ft wide by 6,000 ft long is divided into six equally spaced rows and columns. The transmissivity of the aquifer is 0.08 ft^2/s. Recharge to the aquifer occurs only from stream leakage. The example includes 7 stream segments with totally 16 reaches. There is one diversion (segment 2) and two places where streams join (segments 2 and 4 join to make segment 5 and segments 3, 5, and 6 join to make segment 7). Stream stages are also computed for each reach. The streams range in width from 5 to 10 ft. Streambed conductance values also vary depending on the length and width of each stream reach. The hydraulic conductivity of the streambed deposits is 4 x 10^{-4} ft/s.

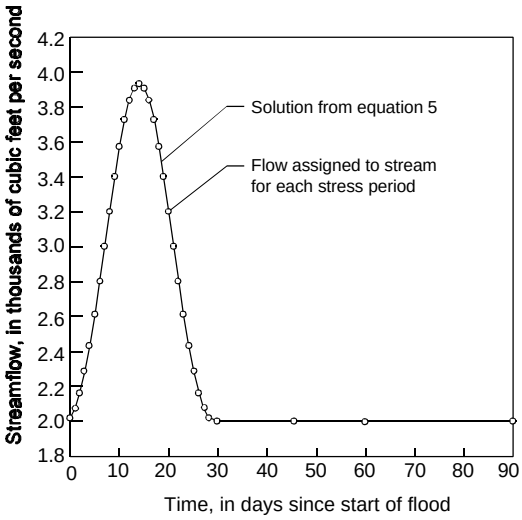


Fig. 6.29 Distribution of streamflow for a 30-day flood event used for the simulation (after Prudic, 1988)

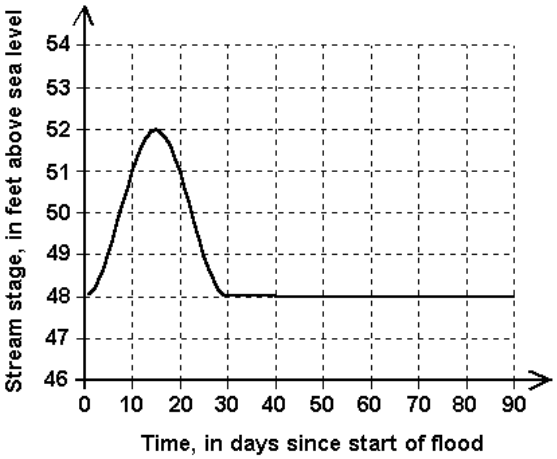


Fig. 6.30 Model calculated river stage

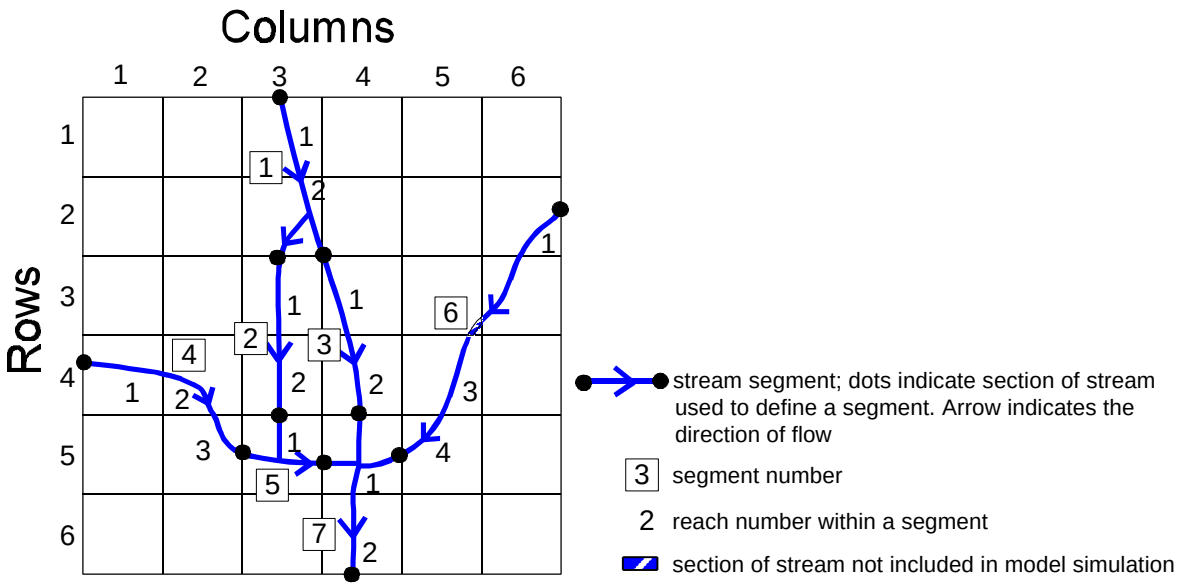


Fig. 6.31 Numbering system of streams and diversions (after Prudic, 1988)

6.2.8 Simulation of Lakes

Folder: \pm5\examples\basic\basic8\

Overview of the Problem

Fig. 6.32 shows an unconfined aquifer with the boundary conditions and the location of a planned open-cast mining site. The aquifer is bounded by a no-flow zone to the north and to the south. To the west and east exist fixed-head boundaries with the hydraulic heads h = 100 m and 95 m; the elevations of the aquifer top and bottom are 100 and 0 m, respectively.

The aquifer is homogeneous and isotropic with a measured horizontal hydraulic conductivity of 0.0001 m/s and vertical hydraulic conductivity of 0.00001 m/s. The specific yield and effective porosity are assumed to be 0.25. The specific storage coefficient S_s = 0.0001. In the final mining phase, the hydraulic head within the mining site must be drawn down to the level of h = 21 m. Afterwards, the mining site will be filled with water to form an artificial lake. Your task is to

1. construct a steady-state flow model and calculate the necessary abstraction rate (= inflow into the mining site) for holding the head at 21 m, and
2. use the calculated steady-state head as the initial hydraulic head and calculate the temporal development curve of the water level (head vs. time) in the artificial lake for the case that the abstraction within the mining site is turned off.

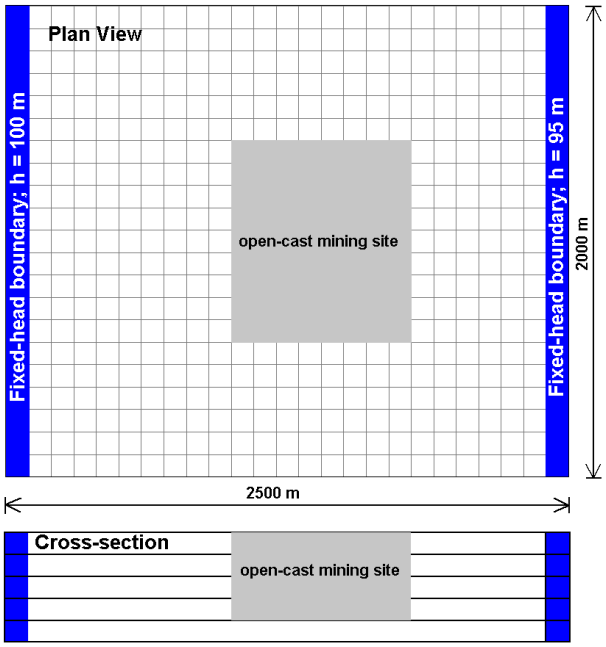


Fig. 6.32 Plan view of the model area

Modeling Approach and Simulation Results

The aquifer is simulated using five model layers, 21 rows and 25 columns. The thickness of each model layer is 20 m. The elevation of the top of the first model layer is 100m. A regular grid spacing of 100 m is used for each column and row. The layer type **3: confined/unconfined (transmissivity varies)** is used for every layer.

For task #1, the cells within the mining site in the 4th model layer are set as fixed-head cells with the initial hydraulic head of 21m. The cells (of all 5 layers) at the west boundary are fixed-head cells with the initial head h = 100m. The cells (of the layers 3 to 5) at the east boundary are fixed-head cells with the initial head h = 50m. The initial hydraulic head at all other cells has been set at 100m. To ensure that there is no resistance to the groundwater flow within the mining site, a very high value (say 1 m/s) is used for the vertical and horizontal hydraulic conductivities of the cells within the site.

A steady-state flow simulation was performed. Fig. 6.33 shows the two cross-sections and the head contours of layer 4. It is obvious that the cells above the groundwater surface went dry. To calculate inflow into the mining site, we select **Tools ▸ Water Budget...** to calculate the water budget by assigning zone 1 to the fixed-heads cells within the mining site. The water budget for zone 1 in layer 4 should look like Table 6.1. The inflow rate to the constant head cells (mining site) is 1.9428713E+00 m^3/s.

Table 6.1 Water budget for the mining site

ZONE 1 IN LAYER 4			
FLOW TERM	IN	OUT	IN-OUT
STORAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
CONSTANT HEAD	0.0000000E+00	1.9428709E+00	-1.9428709E+00
HORIZ. EXCHANGE	1.1840475E+00	0.0000000E+00	1.1840475E+00
EXCHANGE (UPPER)	0.0000000E+00	0.0000000E+00	0.0000000E+00
EXCHANGE (LOWER)	7.5882387E-01	0.0000000E+00	7.5882387E-01
WELLS	0.0000000E+00	0.0000000E+00	0.0000000E+00
DRAINS	0.0000000E+00	0.0000000E+00	0.0000000E+00
RECHARGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
ET	0.0000000E+00	0.0000000E+00	0.0000000E+00
RIVER LEAKAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
HEAD DEP BOUNDS	0.0000000E+00	0.0000000E+00	0.0000000E+00
STREAM LEAKAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
INTERBED STORAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
SUM OF THE LAYER	1.9428713E+00	1.9428709E+00	4.7683716E-07

For task #2, all cells within the mining site are set as active cells. The wetting capability of MODFLOW is turned on by selecting **Models ▸ Modflow▸Wetting Capability...**. The wetting-iteration interval is 1, wetting factor is 0.5 and THRESH is -1 for all cells. The specific yield and

effective porosity of all cells within the mining site (lake) are set to 1. Compared to the specific yield, the influence of the confined storage coefficient within the lake is very small and can normally be ignored. Therefore, the specific storage coefficient S_s = 0.0001 is assigned to all cells. A transient flow simulation is performed for a stress period with the length of 3.15576E+08 seconds, 100 time steps and a time-step multiplier of 1.0. The temporal development curve of the water table at the a borehole, which is located in the fourth layer within the lake, is shown in Fig. 6.34. The final stage in the lake is about 97.1 m.

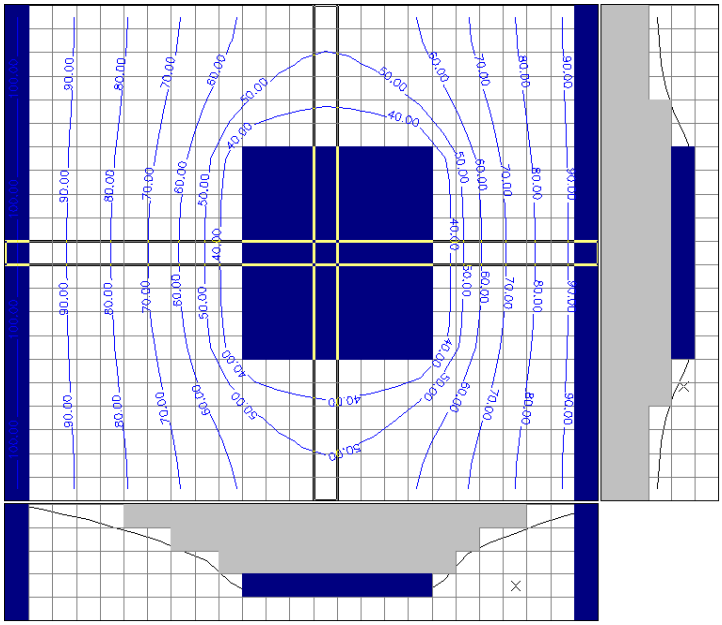


Fig. 6.33 Head contours in layer 4

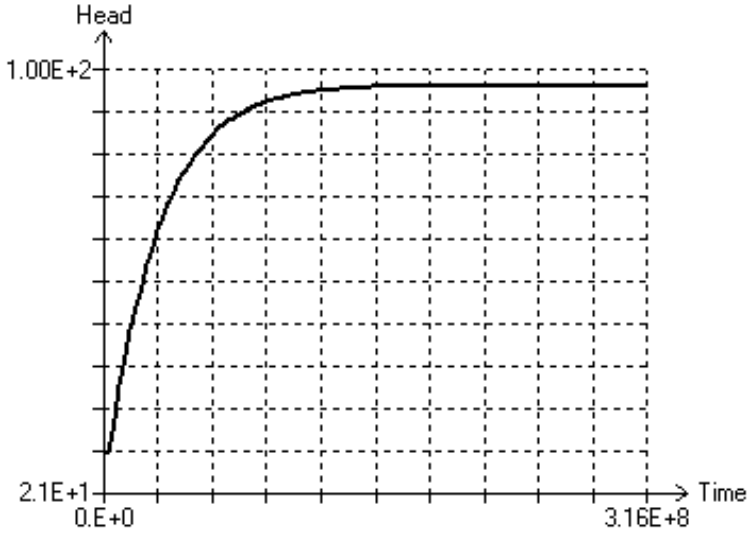


Fig. 6.34 Temporal development curve of the water stage in the artificial lake

6.3 EPA Instructional Problems

Folder: \pm5\examples\EPA Instructional Problems\

Overview of the Problems

The manual of instructional problems for MODFLOW (Andersen, 1993) is intended to allow the student to have hands-on experience with the practical application of models. Twenty documented problems, complete with problem statements, input data sets, and discussion of results are presented in that manual. The problems are designed to cover modeling principles, specifics of input/output options available to the modeler, rules of thumb, and common modeling mistakes. You can find an electronic version of this manual in the folder \Documents\Instructional Problems for MODFLOW (EPA) on the companion CD-ROM.

Modeling Approach and Simulation Results

We have rebuilt most of the models described in the manual of instructional problems. If you have selected to install the Example Pack *EPA instructional problems* during the installation of PMWIN, you can find the models in sub-folders under \pm5\examples\EPA Instructional Problems\. Although these models are ready-to-run, it is suggested to construct the models by yourself, because one will learn more through mistakes and exercises.

6.4 Automatic Calibration and Pumping Test

6.4.1 Basic Model Calibration Skill with PEST/UCODE

Folder: \pm5\examples\calibration\calibration1\

Overview of the Problem

Groundwater models are usually applied to conceptualize and understand a hydrologic system or to predict the outcome of a future change to the system. In order to provide some assurance that the model reflects the behavior or appearance of the flow system, it must be calibrated prior to use as a predictive tool. Calibration is accomplished by finding a set of parameters, boundary conditions, and excitations or stresses that produce simulated heads (or drawdowns) and fluxes that match measurement values within an acceptable range of error. Model calibration can be performed by the hand-operated trial-and-error adjustment of aquifer parameters or by inverse models such as PEST, UCODE, MODINV (Doherty, 1990) or MODFLOW/P (Hill, 1992). This example provides an exercise in model calibration with PEST and UCODE. Specific details of this example are from Andersen (1993).

Fig. 6.35 shows the idealized flow system and locations of observation bores. The flow system is a small, confined aquifer which is strongly controlled by the river which is flowing across it. The aquifer is approximately 100 ft thick and is composed primarily of silty sand. The river is not in direct hydraulic connection with the aquifer, but acts as a leaky boundary condition which can gain or lose water to the aquifer. Stage data for the river and riverbed elevation are listed in Table 6.2. Other boundary conditions are no-flow, which surround the square and define the areal extent of the aquifer.

Given constraints of uniform transmissivity and recharge, and additional data below, obtain a steady state calibration based on the measurements listed in Table 6.3.

Initial hydraulic head = 100.0 ft
grid size = 15× 15
$\Delta x = \Delta y = 500$ ft
river base flow at western model boundary = 10 cfs
river base flow at eastern model boundary = 11.125 cfs
riverbed conductance = 0.01 ft^2/s

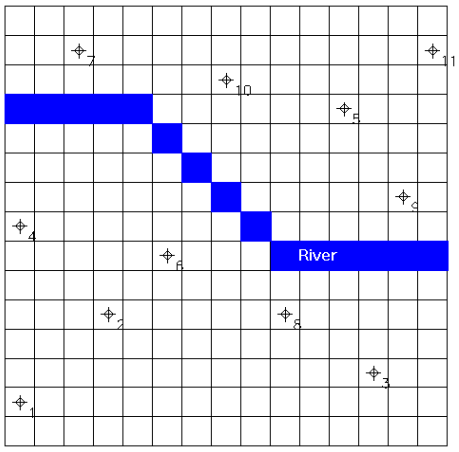


Fig. 6.35 Configuration of the aquifer system

Table 6.2 River data

Row	Column	Stage (ft)	Riverbed Elevation (ft)
4	1	100.0	90.0
4	2	100.0	90.0
4	3	100.0	90.0
4	4	99.0	89.0
4	5	99.0	89.0
5	6	98.0	88.0
6	7	97.0	86.0
7	8	96.0	86.0
8	9	95.0	85.0
9	10	94.0	84.0
9	11	94.0	84.0
9	12	94.0	84.0
9	13	94.0	84.0
9	14	93.0	83.0
9	15	93.0	83.0

Table 6.3 Measurement data

Bore	Row	Column	Head (ft)
1	14	1	124.0
2	11	4	119.9
3	13	13	113.9
4	8	1	116.1
5	4	12	113.0
6	9	6	114.0
7	2	3	108.5
8	11	10	111.7
9	7	14	107.6
10	3	18	111.3
11	2	15	115.6

Modeling Approach and Simulation Results

The aquifer is simulated using a grid of one layer, 15 columns and 15 rows. A regular grid space of 500 ft is used for each column and row. The layer type is **0:confined** and the **Transmissivity** flag in the **Layer Options** dialog box is **user-specified**. Transmissivity and recharge are defined as estimated parameters with the parameter numbers 1 and 2 (Note that the names of these two parameters are p1 and p2).

Table 6.4 shows the optimized parameter values and the correlation coefficient matrix calculated by PEST. A similar result obtained by UCODE is shown in Table 6.5. The diagonal elements of the correlation coefficient matrix are always unity. The off-diagonal elements are always between 1 and -1. The closer an off-diagonal element is to 1 or -1, the more highly correlated are the parameters corresponding to the row and column numbers of that element. For this example, transmissivity (parameter p1) and recharge (parameter p2) are highly correlated, as is indicated by the value 0.9572 of the correlation coefficient matrix. This means that these parameters are determined with a high degree of uncertainty in the parameter estimation process. A sensitivity analysis could be used to quantify the uncertainty in the calibrated model caused by uncertainty in the estimates of the aquifer parameters.

For our example, the only discharge is to the river and the only source is recharge. To be in steady state, these two must balance. Recharge must therefore be equal to 1.125 cfs (the river gain equals 11.125 cfs - 10 cfs). Spreading over the modeled area:

$$recharge = \frac{1.125 ft^3/s}{(15 \times 15)\cdot(500 ft \times 500 ft)} = 2\times10^{-8}\ ft/s \qquad (6.1)$$

The estimated parameter values are acceptable. A better procedure would have been to compute the recharge right-away from eq. (6.1) and calibrate only transmissivity.

Table 6.4 Optimized parameter values and the correlation coefficient matrix. Calibration result from PEST.

```
Parameter      Estimated          95% percent confidence limits
               value              lower limit       upper limit
 p1           1.000282E-02        9.724991E-03      1.028859E-02
 p2           1.996080E-08        1.985581E-08      2.006578E-08

Note: confidence limits provide only an indication of parameter uncertainty.
      They rely on a linearity assumption which  may not extend as far in
      parameter space as the confidence limits themselves - see PEST manual.

Correlation Coefficient Matrix ----->
  1.000       0.9572
 0.9572        1.000
```

Table 6.5 Optimized parameter values and the correlation coefficient matrix. Calibration result from UCODE.

```
PARAMETER ID:            P1          P2

UPPER 95% C.I.     1.01E-02    2.01E-08
FINAL VALUES       1.00E-02    2.00E-08
LOWER 95% C.I.     9.90E-03    1.98E-08

          ----------------
          CORRELATION MAT.
          ----------------

            1           2
.............................
  1     1.000      0.9869
  2    0.9869       1.000
```

6.4.2 Estimation of Pumping Rates

Folder: \pm5\examples\calibration\calibration2\

Overview of the Problem

This example involves the encapsulation of a highly contaminated area. The aquifer in which the contaminated area is buried is unconfined, isotropic and of infinite areal extent. The extent of the contamination area is about 65 m × 65 m. The head in the center of this area is about 9.45 m. The elevation of the aquifer top is 10 m and the aquifer bottom is at 0 m. The hydraulic conductivity is uniformly 3×10^{-4} m/s. The unconfined storage coefficient (specific yield) is 0.2. Recharge is assumed to be zero. The groundwater flow is directed from west to east with a hydraulic gradient of 0.5‰.

To prevent contaminated water flow out of the area, a remediation measure is required. Different types and combinations of measures can be introduced for this purpose including a cut-off wall around the area, drainages and pumping wells. All measures are directed towards the same goal - a reduction of the piezometric head in the contaminated area itself such that groundwater flows towards the contaminated area. To achieve this objective, a cut-off wall around this area and four pumping wells have been chosen. The cut-off wall is 0.5 m thick and the hydraulic conductivity of the material is 5×10^{-8} m/s.

Your task is to estimate the required pumping rate of the wells such that the steady-state piezometric head in the center of the contaminated area is 8 m. Furthermore, the duration until the steady-state is reached should be calculated.

Modeling Approach and Simulation Results

The aquifer is simulated using a grid of one layer, 31 columns and 31 rows. The layer type is **1:unconfined**. Fig. 6.36 shows the model grid and the selected boundary conditions. The extent of the model is fairly large. To obtain the hydraulic gradient of 0.5‰, the west and east sides of the model are assumed to be fixed-head boundaries with hydraulic heads of 9.8925 and 9 m, respectively.

The configuration of the remediation measures is shown in Fig. 6.37. The pumping rates of the wells are defined as an estimated parameter by assigning the parameter number 1 to all four wells. An "observation" borehole is set at the center of the contaminated area. The "observed" head at time 1 is set at 8 m (the remediation objective) in the **Boreholes and Observations** dialog box. The simulation time is also set to 1. Using PEST or UCODE, the pumping rate of

each well is estimated at about 7.9×10^{-5} m^3/s.

To calculate the duration until the steady-state is reached, the estimated pumping rate of 7.9×10^{-5} m^3/s is specified to each well. A transient simulation with one stress period (subdivided into 25 equal time steps) is carried out. The total simulation time is 1×10^{8} seconds. The calculated head-time curve (Fig. 6.38) shows that the steady-state is reached at $t\approx4\times10^{7}$ s.

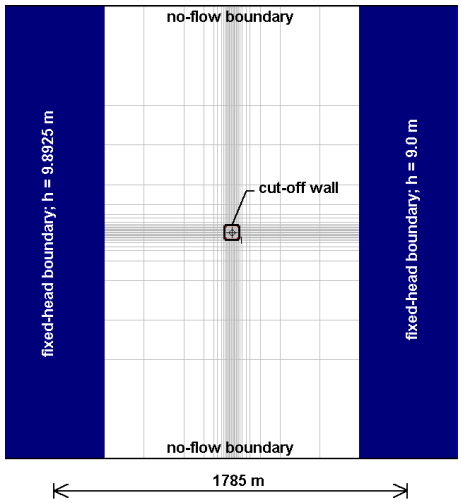


Fig. 6.36 Plan view of the model

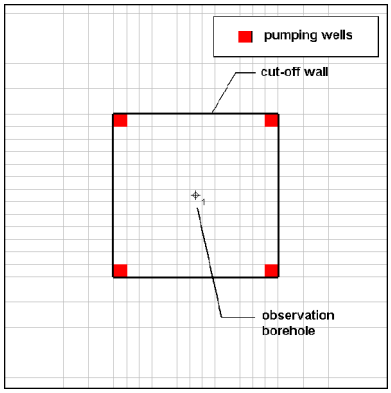


Fig. 6.37 Location of the cut-off wall and pumping wells

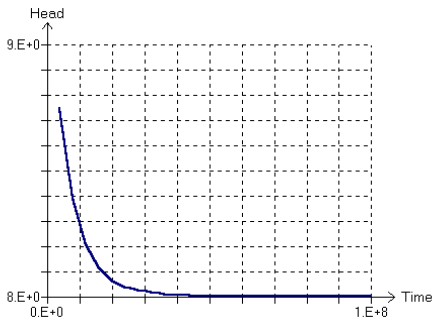


Fig. 6.38 Head versus time at the center of the contaminated area

6.4.3 The Theis Solution - Transient Flow to a Well in a Confined Aquifer

Folder: \pm5\examples\calibration\calibration3\

Overview of the Problem

This example gives an approximation of the Theis solution with a numerical model. Given the aquifer properties, transmissivity and confined storage coefficient, the Theis solution predicts drawdown in a confined aquifer at any distance from a well at any time since the start of pumping. The assumptions inherent in the Theis solution include:

(1) The aquifer is homogeneous, isotropic and of uniform thickness,
(2) The aquifer is confined between impermeable formation on top and bottom, and of infinite areal extent.
(3) The initial piezometric surface is horizontal and uniform.
(4) The pumping rate of the well is constant with time.
(5) The well penetrates the entire aquifer and the well diameter is small.
(6) Water is removed from storage instantaneously with decline in head.

All of these assumptions, with the exception of infinite areal extent, can be represented by a numerical model.

In this example, a fully penetrating well is located at the center of the model domain and withdraws water at a constant rate. The drawdown of the hydraulic head is monitored with time at a borehole 55m from the pumping well. The model parameters are listed below. Your task is to construct a numerical model, calculate the drawdown curve at the borehole and compare it with the analytical (Theis) solution.

Initial hydraulic head = 0.0 m
Transmissivity = 0.0023 m^2/s
Storage coefficient = 0.00075
Pumping rate = 4×10^{-3} m^3/s
Total simulation time = 86400 s
Number of time steps = 20
Time step multiplier = 1.3
Number of SIP iteration parameters = 5
Convergence criterion of head change = 0.0001 m
Maximum number of iterations = 50

Modeling Approach and Simulation Results

To meet the requirement of an infinite areal extent, the modelled domain is chosen fairly large (The boundary could alternatively be moved even further from the pumping well by using the General Head Boundary, see section 6.2.2). The aquifer is simulated by a single layer model. An increasing grid spacing expansion is used to extend the model boundaries (Fig. 6.39). The layer type is **0:confined.** In the **Layer Options** dialog box, the flags of **Transmissivity** and **Storage Coefficient** are set to **User-specified**. The top and bottom elevations of the model layer are not required.

The analytical drawdown values at the borehole are specified in the **Boreholes and Observations** dialog box. Both the analytical and calculated drawdown curves are shown in Fig. 6.40. An exact comparison is not attained because of the approximations made in the numerical model. These include: (1) use of a discrete rather than continuous spatial domain, (2) use of a discrete rather than continuous time domain, (3) use of an iterative solution with a convergence tolerance, and (4) artificial placement of boundaries.

In practice, you can use this model to estimate transmissivity and confined storage coefficient by specifying the real observation time and data in the **Boreholes and Observations** dialog box. By defining transmissivity and storage coefficient as estimated parameters, the inverse models PEST or UCODE can estimate the parameters automatically. Click **Models ▸ PEST ▸ Run...** or **Models ▸ UCODE ▸ Run...** to see how the inverse models work. Because the analytical drawdown values were used as the observations, the results from the inverse models must be transmissivity = 0.0023 m^2/s and storage coefficient = 0.00075.

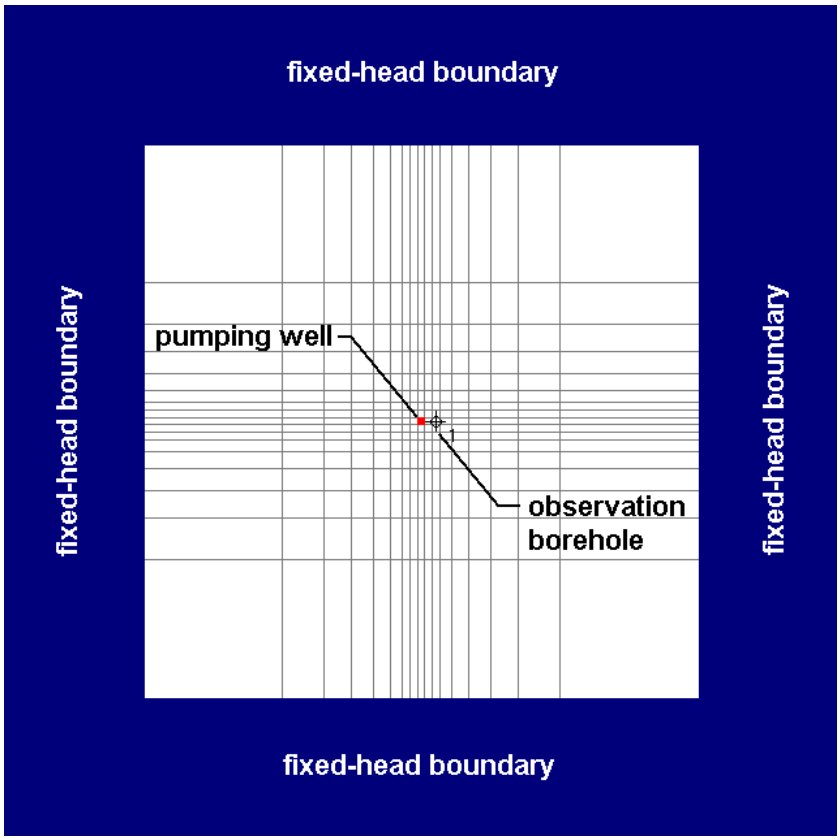


Fig. 6.39 Configuration of the groundwater model

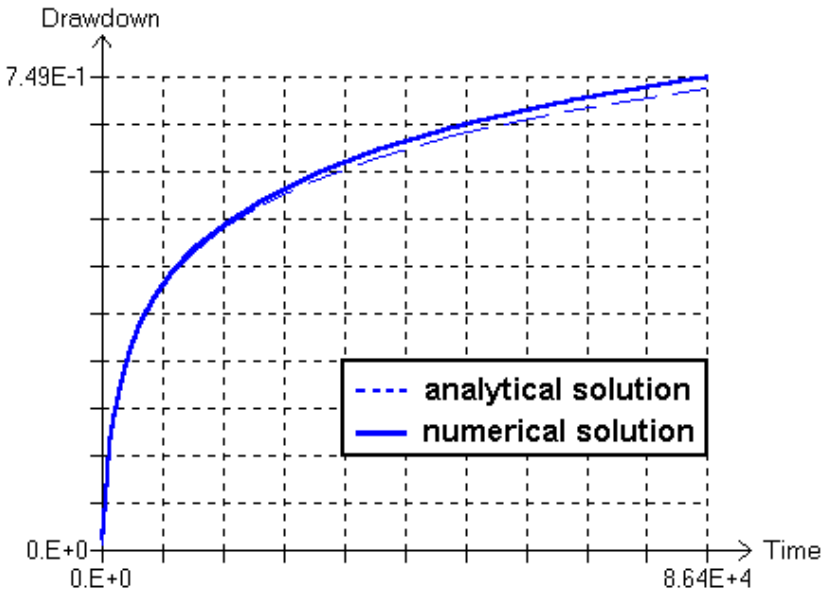


Fig. 6.40 Drawdown-time curves

6.4.4 The Hantush and Jacob Solution - Transient Flow to a Well in a Leaky Confined Aquifer

Folder: \pm5\examples\calibration\calibration4\

Overview of the Problem

This examples demonstrates how to approach leaky confined aquifers. A leaky confined aquifer is overlaid and/or underlaid by geologic formations, which are not completely impermeable and can transmit water at a sufficient rate (Fig. 6.41). Hantush and Jacob (1955) give an analytical solution to describe the drawdown with time during pumping with a well in a leaky confined aquifer. In addition to the assumptions in the Theis solution, the analytical solution requires two assumptions - the hydraulic head in the overlying oder underlying aquifer is constant during pumping in the leaky confined aquifer and the rate of leakage into the pumped aquifer is proportional to drawdown.

In this example, a pumping well withdraws water at a constant rate from the leaky confined aquifer. The drawdown of the hydraulic head is monitored with time at a borehole 55m from the pumping well. The borehole is located in the leaky confined aquifer. The initial hydraulic head is 8 m everywhere. Specific yield and effective porosity are 0.1. The other aquifer parameters are given in Fig. 6.41. The analytical solution for this case is given in Table 6.6.

Your task is to construct a numerical model, calculate the drawdown curve at the borehole and compare it with the Hantush-Jacob solution. Note that the parameters for the confined leaky aquifer are the same as in the previous example, so we can compare the results of these two examples.

Table 6.6 Analytical solution for the drawdown with time

Time (s)	drawdown (m)	Time (s)	drawdown (m)
123	0.0067	4932	0.336
247	0.03	12330	0.449
352	0.052	24660	0.529
493	0.077	35228	0.564
1233	0.168	49320	0.595
2466	0.25	123300	0.652
3523	0.294		

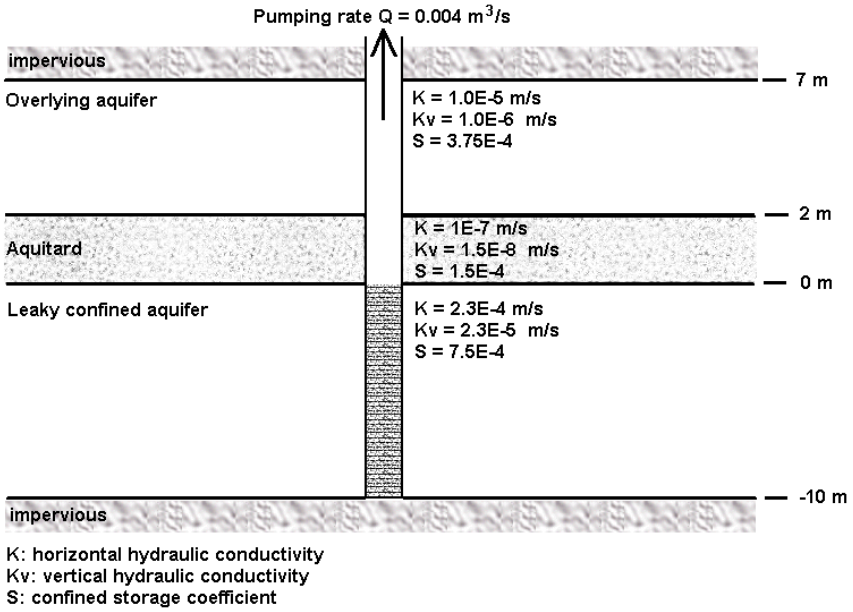


Fig. 6.41 Configuration of the leaky aquifer system and the aquifer parameters

Modeling Approach and Simulation Results

The modelled domain is the same as in the previous example. Three model layers are used to simulate the system. The layer types are **3:confined/unconfined (transmissivity varies).** In the **Layer Options** dialog box, the **Storage Coefficient** flag is set to **user-specified** and the **Transmissvity** flag is **calculated**. All model cells in the first model layer are fixed-head cells and all other cells are specified as active cells. A transient flow simulation is performed for a stress period with the length of 49320 seconds, 20 time steps and a time-step multiplier of 1.3. For comparison, the analytical solution is entered in the **Boreholes and Observations** dialog box. Fig. 6.42 shows the numerical and analytical drawdown-time curves at the observation borehole, which is at a distance of 55 m from the pumping well. The match of these two curves is very good.

While the use of the analytical solution is limited to the primary assumptions, the numerical model can be used to evaluate pumping tests, even if the confining aquitard (Fig. 6.41) has a higher value of the vertical hydraulic conductivity and the hydraulic head in the overlying aquifer is not constant during the pumping. To do this, simply specify all model cells as active cells. This is allowed because the simulation time is normally very short and the extent of the model domain is relative large, so that at end of a transient flow simulation the drawdown values at the model boundaries are acceptable low.

If the vertical hydraulic conductivity of the aquitard is known, we can use PEST or UCODE

to estimate the horizontal hydraulic conductivity and storage coefficient of the leaky aquifer by defining them as estimated parameters. Click **Models ▸ PEST ▸ Run...** or **Models ▸ UCODE ▸ Run...** to see how the inverse models work. Because the analytical drawdown values were used as the observations, the results from the inverse models must be horizontal hydraulic conductivity ≈ 2.3×10^{-4} m/s and storage coefficient ≈ 0.00075. If the vertical hydraulic conductivity is unknown and needs to be estimated, we will need additional drawdown values in the overlying aquifer during the pumping test.

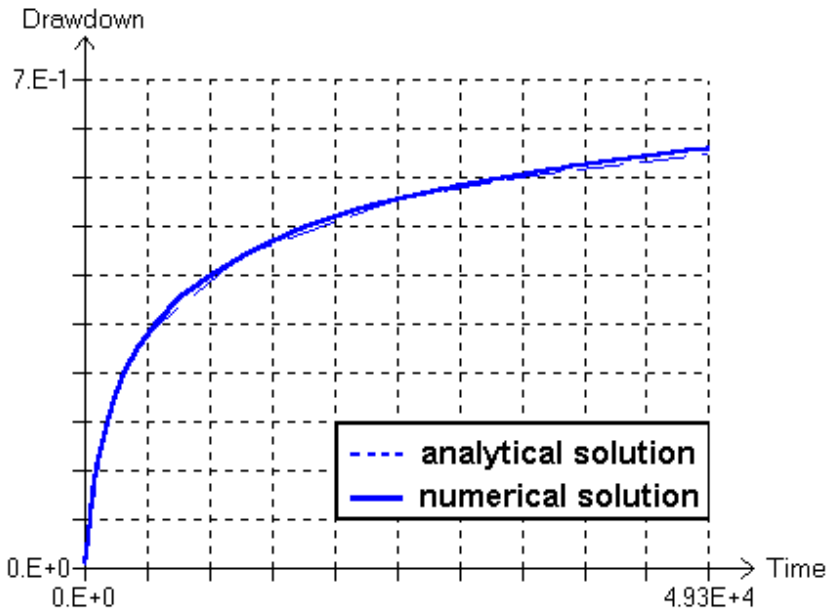


Fig. 6.42 Drawdown-time curves

6.5 Geotechnical Problems

6.5.1 Inflow of Water into an Excavation Pit

Folder: \pm5\examples\geotechniques\geo1\

Overview of the Problem

This example is adopted from Kinzelbach and Rausch (1995). Fig. 6.43 shows a plan view and a cross section through a shallow aquifer situated in a valley. In the north the aquifer is bounded by the outcrop of the sediments in the valley, while the south boundary is a river, which is in contact with the aquifer. The aquifer extends several kilometers to the west and east, it is unconfined, homogeneous and isotropic. The top and bottom elevations of the aquifer are 7 m and 0 m, respectively. The average horizontal hydraulic conductivity of the sandy sediments is 0.001 m/s; the effective porosity is 0.15. The groundwater recharge from precipitation is 6×10^{-9} $m^3/s/m^2$. The water stage in the river is 5 m above the flat aquifer bottom, which is the reference level for the simulation. At a distance of 200 m from the river there is an excavation pit. The length of the pit is 200 m, the width 100 m. The bottom of the excavation is 3 m above the aquifer bottom.

Your task is to calculate the inflow into the pit and show head contours and catchment area of the pit.

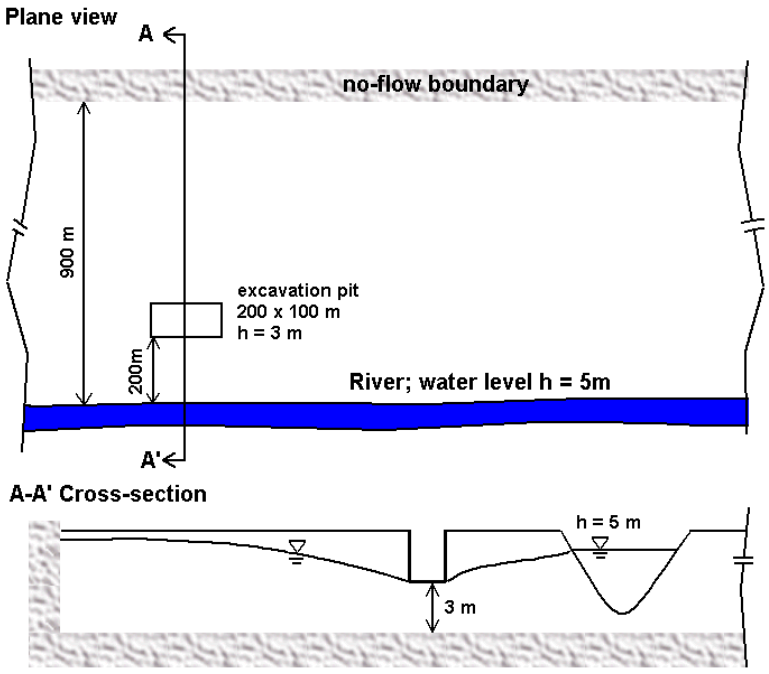


Fig. 6.43 Problem description

Modeling Approach and Simulation Results

The aquifer is simulated using a grid of one layer, 40 columns and 19 rows. A regular grid spacing of 50 m is used for each column and row. The layer type is **1:unconfined**. To simplify the simulation, use of symmetry is made by modeling only half the domain. The river and the pit are modelled as fixed-head boundaries with hydraulic heads of h = 5 m and 3 m, respectively. All other boundaries are no-flow boundaries. The distance between the eastern no-flow boundary and the pit is not known a priori and must be selected large enough so that it is not influenced by the pit. Fig. 6.44 shows the head contours, the catchment area of the excavation and two cross-sections. Using the Water budget calculator, the inflow into the pit is calculated at 2 × 0.0129 m^3/s = 0.0258 m^3/s.

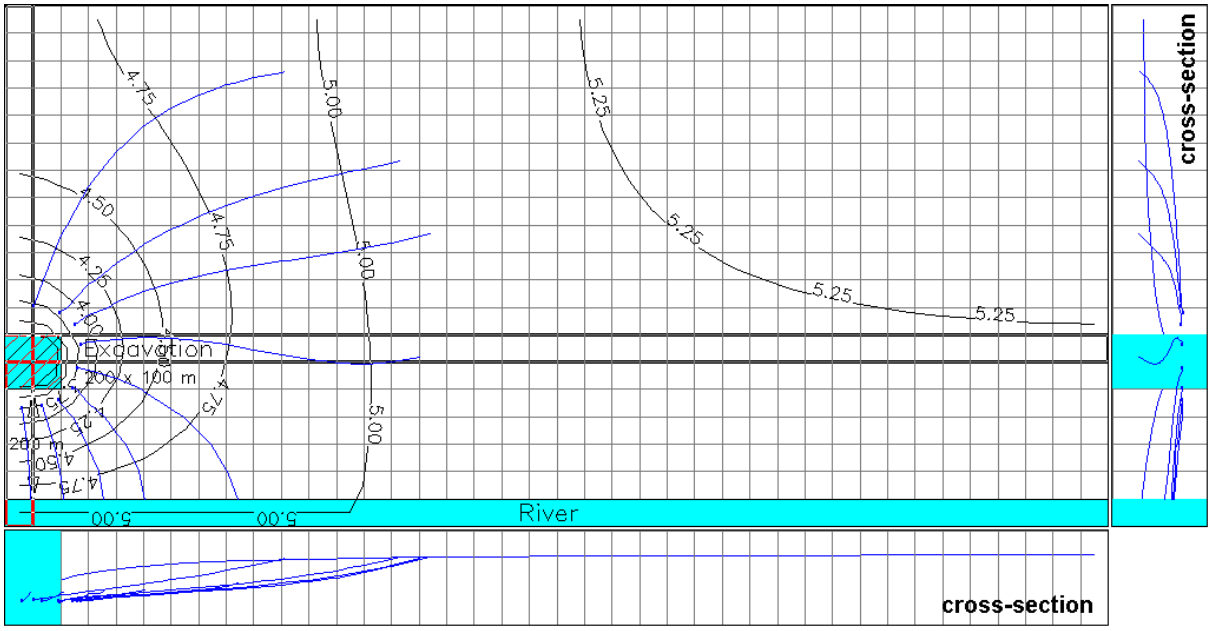


Fig. 6.44 Simulated head distribution and catchment area of the excavation pit

6.5.2 Flow Net and Seepage under a Weir

Folder: \pm5\examples\geotechniques\geo2\

Overview of the Problem

This example is adopted from Kinzelbach and Rausch (1995). An impervious weir is partially embedded in a confined aquifer. The aquifer is assumed to be homogeneous with a hydraulic conductivity of the aquifer of 0.0005 m/s and a thickness of 9 m. The effective porosity of the aquifer is 0.15. The boundary conditions are shown in Fig. 6.45. Calculate the flow net and the flux through the aquifer for the cases that (1) the aquifer is isotropic and (2) the aquifer is anisotropic with an anisotropy factor of 0.2.

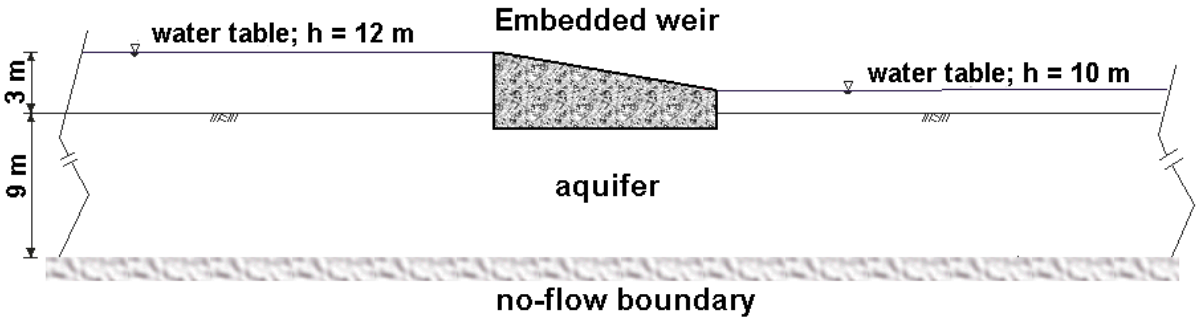


Fig. 6.45 Problem description

Modeling Approach and Simulation Results

To compute the head distribution and the corresponding flowlines it is sufficient to consider a vertical cross-section of the aquifer with a uniform thickness of 1 m. The aquifer is simulated using a grid of one layer, 65 columns and 9 rows. A regular grid spacing of 1 m is used for each column and row. The layer type is **0:confined**. Fig. 6.46 shows the cross section, the selected model grid and the boundary conditions. The boundaries at the upstream and downstream of the weir are modeled as fixed-head boundaries with h = 12 m and h = 10 m above reference level, respectively. The aquifer bottom and the weir itself are modelled as no-flow boundaries.

Fig. 6.47 shows the flow net for the isotropic case. The head values range from 10 to 12 m with a head increment of 0.1 m. The flux through the aquifer (per m width of the weir) is 3.65×10^{-4} $m^3/s/m$ ($\approx$31.56 $m^3/day/m$). Fig. 6.48 shows the flow net for the aquifer in the

anisotropic case. The flux through the aquifer is now only 2.5×10^{-4} $m^3/s/m$ ($\approx$21.6 $m^3/day/m$). Note that in a homogeneous and anisotropic medium, flowlines intersect head contours at right angle only where flow is parallel to one of the principal directions of hydraulic conductivity.

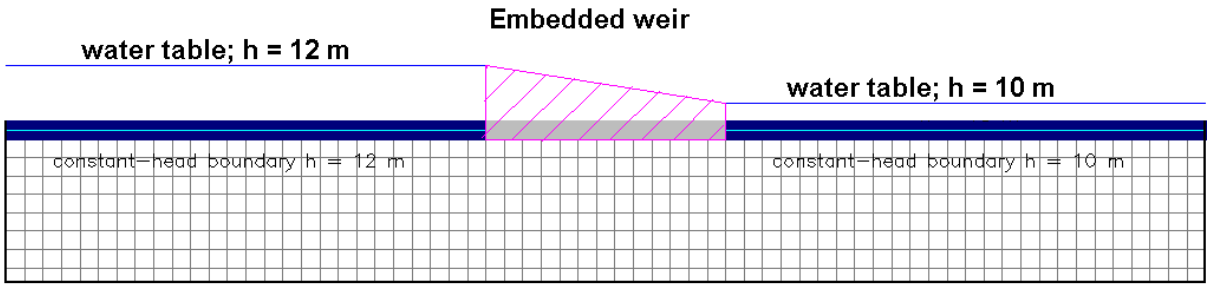


Fig. 6.46 Model grid and the boundary conditions

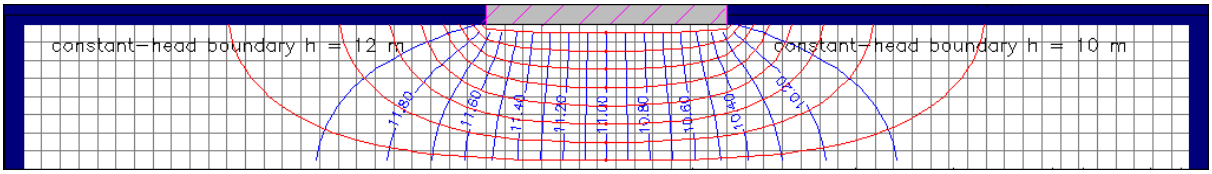


Fig. 6.47 Flowlines and calculated head contours for isotropic medium

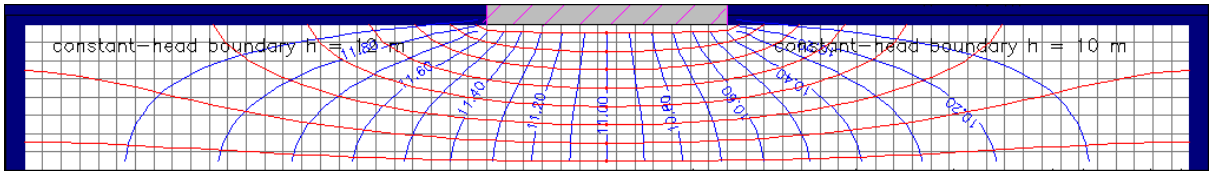


Fig. 6.48 Flowlines and calculated head contours for anisotropic medium

6.5.3 Seepage Surface through a Dam

Folder: \pm5\examples\geotechniques\geo3\

Overview of the Problem

This example is adopted from Kinzelbach and Rausch (1995). This example demonstrates how to calculate the seepage surface using a vertical cross-sectional model. As shown in Fig. 6.49, the length of the dam is 100 m, the thickness and height are 10m. The water table is 10 m at the upstream side of the dam and 2 m at the downstream side. The material of the dam is homogeneous and isotropic with a hydraulic conductivity of 1×10^{-5} m/s. The unrealistic bank slope is used here to simplify the data input.

Your task is to calculate the seepage surface and the seepage rate by using a vertical cross-sectional numerical model. Compare the seepage rate with an analytical solution after Dupuit.

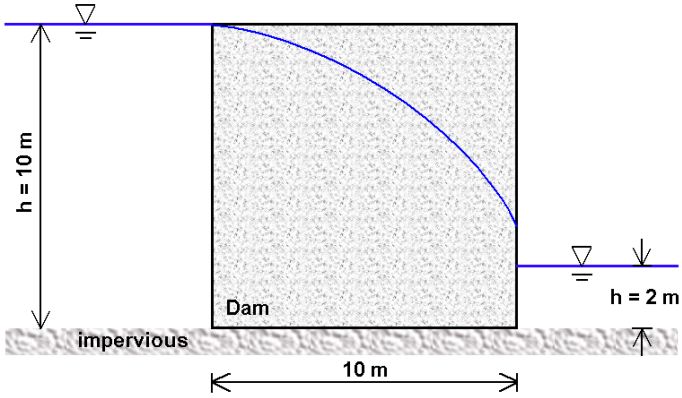


Fig. 6.49 Seepage surface through a dam

Modeling Approach and Simulation Results

To compute the head distribution and the seepage surface, it is sufficient to consider a vertical cross-section of the aquifer with a uniform thickness of 1 m. The aquifer is simulated using a grid of one layer, 21 columns and 20 rows. A regular grid spacing of 0.5 m is used for each column. The layer type is **0:confined**. The boundary at the upstream side of the dam is modeled as fixed-head boundary with the hydraulic head h = 10 m. On the right-hand side of the dam, there are four fixed-head cells with h = 2 m. The other cells on this boundary are modelled as drain cells with a high *drain hydraulic conductance* $[L^2T^{-1}]$ value. The elevation of the drain is set the same as the bottom elevation of each cell, for example the 2.0 m for the cell [21, 16, 1] and 2.5 m for the cell [21, 15, 1]. The drain cells are activated only if water table is higher than the level of the

drain. The selected model grid and the boundary conditions are shown in Fig. 6.50. Except the four fixed-head cells at the right-hand side of the dam, the initial hydraulic head for all cells are 10 m.

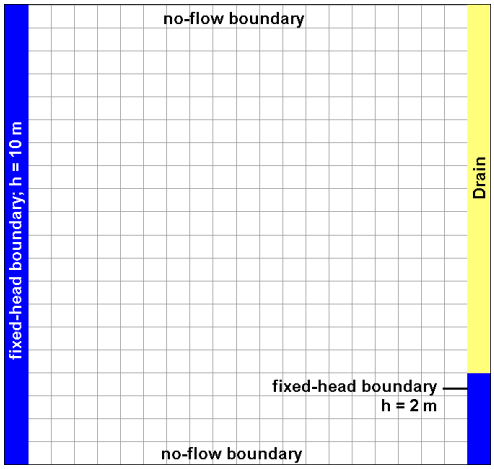


Fig. 6.50 Model grid and the boundary conditions

The first step in solving this problem is to carry out a steady-state flow simulation with these data. Fig. 6.51 shows the calculated hydraulic heads. By comparing the calculated heads with the elevation of the cell bottom, we can easily find that the hydraulic heads of some of the cells at the upper-right corner of the model are lower than the cell bottom. This means that these cells went dry. In the second step, these dry cells will be defined as inactive cells by setting IBOUND = 0 and a steady-state flow simulation will be carried out again. Now, it is possible that some of the calculated heads are higher than the top elevation of the highest active cell. In this case, these cells will be defined as active and a steady-state flow simulation will be performed again. This iterative solution will be repeated until the water table remains unchanged between two iteration steps. Fig. 6.52 shows the calculated head distribution and the form of the seepage surface. The seepage rate is about 4.8×10^{-5} $m^3/s/m$ and the total seepage rate through the dam (lenght 100 m) is 4.8×10^{-3} m^3/s.

The analytical solution of the seepage rate after the Dupuit assumption is

$$Q = K \cdot B \cdot \frac{(h_1^2 - h_2^2)}{2L} = K \cdot \frac{h_1 + h_2}{2} \cdot B \cdot \frac{h_1 - h_2}{L} \qquad (6.2)$$

where B is the length of the dam, L is the thickness of the dam, K is the hydraulic conductivity, h_1 and h_2 are the heads at the uptream and downstream sides of the dam, respectively. The modified form of the analytical solution is Darcy's Law with a mean transmissivity of $K (h_1 + h_2)/2$. For this example with h_1= 10 m, h_2 = 2 m, L = 10 m, B = 100 m and $K = 1 \times 10^{-5}$ m/s, the seepaga rate Q is exactly equal to 4.8×10^{-3} m^3/s.

Cells in the J-direction

Cells in the I-direction	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	elevation of the cell bottom [m]
1	10	9.75	9.50	9.25	9.01	8.77	8.54	8.31	8.08	7.86	7.66	7.46	7.27	7.10	6.94	6.80	6.68	6.58	6.51	6.46	6.43	9.5
2	10	9.75	9.50	9.25	9.01	8.77	8.53	8.30	8.07	7.86	7.65	7.45	7.26	7.08	6.92	6.78	6.66	6.56	6.48	6.43	6.40	9.0
3	10	9.74	9.50	9.25	9.00	8.76	8.52	8.29	8.06	7.84	7.63	7.42	7.23	7.05	6.89	6.74	6.62	6.51	6.43	6.38	6.35	8.5
4	10	9.74	9.49	9.24	8.99	8.75	8.51	8.27	8.04	7.81	7.60	7.39	7.19	7.01	6.84	6.69	6.55	6.44	6.36	6.30	6.27	8.0
5	10	9.74	9.49	9.23	8.98	8.73	8.49	8.24	8.01	7.78	7.56	7.34	7.14	6.95	6.77	6.61	6.47	6.35	6.26	6.19	6.16	7.5
6	10	9.74	9.48	9.22	8.97	8.71	8.46	8.22	7.97	7.74	7.51	7.29	7.07	6.87	6.68	6.51	6.36	6.23	6.13	6.05	6.02	7.0
7	10	9.73	9.47	9.21	8.95	8.69	8.44	8.18	7.93	7.69	7.45	7.22	7.00	6.78	6.58	6.40	6.23	6.08	5.96	5.88	5.83	6.5
8	10	9.73	9.46	9.20	8.93	8.67	8.40	8.15	7.89	7.64	7.39	7.15	6.91	6.68	6.46	6.26	6.07	5.91	5.77	5.67	5.61	6.0
9	10	9.72	9.45	9.18	8.91	8.64	8.37	8.11	7.84	7.58	7.32	7.06	6.81	6.57	6.33	6.11	5.90	5.70	5.54	5.41	5.33	5.5
10	10	9.72	9.44	9.16	8.89	8.61	8.34	8.06	7.79	7.52	7.25	6.98	6.71	6.45	6.19	5.94	5.70	5.48	5.27	5.09	4.97	5.0
11	10	9.71	9.43	9.15	8.87	8.58	8.30	8.02	7.74	7.46	7.17	6.89	6.61	6.33	6.05	5.77	5.50	5.23	4.97	4.72	4.50	4.5
12	10	9.71	9.42	9.13	8.85	8.56	8.27	7.98	7.69	7.39	7.10	6.80	6.50	6.20	5.90	5.59	5.28	4.97	4.65	4.33	4.00	4.0
13	10	9.70	9.41	9.12	8.82	8.53	8.23	7.94	7.63	7.33	7.03	6.71	6.40	6.08	5.75	5.42	5.08	4.72	4.35	3.94	3.50	3.5
14	10	9.70	9.40	9.10	8.81	8.50	8.20	7.90	7.59	7.27	6.96	6.63	6.30	5.96	5.61	5.25	4.88	4.49	4.07	3.60	3.00	3.0
15	10	9.69	9.39	9.09	8.79	8.48	8.17	7.86	7.54	7.22	6.89	6.56	6.21	5.86	5.49	5.10	4.70	4.28	3.84	3.39	3.00	2.5
16	10	9.69	9.39	9.08	8.77	8.46	8.15	7.83	7.50	7.17	6.84	6.49	6.13	5.76	5.38	4.97	4.54	4.09	3.62	3.13	2.71	2.0
17	10	9.69	9.38	9.07	8.76	8.44	8.13	7.8	7.47	7.14	6.79	6.43	6.07	5.68	5.28	4.86	4.41	3.93	3.40	2.80	2.0	1.5
18	10	9.69	9.37	9.06	8.75	8.43	8.11	7.78	7.45	7.11	6.75	6.39	6.02	5.62	5.21	4.78	4.31	3.81	3.27	2.67	2.0	1.0
19	10	9.68	9.37	9.06	8.74	8.42	8.10	7.77	7.43	7.09	6.73	6.36	5.98	5.58	5.16	4.72	4.25	3.74	3.20	2.61	2.0	0.5
20	10	9.68	9.37	9.06	8.74	8.42	8.09	7.76	7.42	7.07	6.72	6.35	5.96	5.56	5.14	4.69	4.21	3.71	3.17	2.59	2.0	0.0

Fig. 6.51 Calculated hydraulic heads after one iteration step

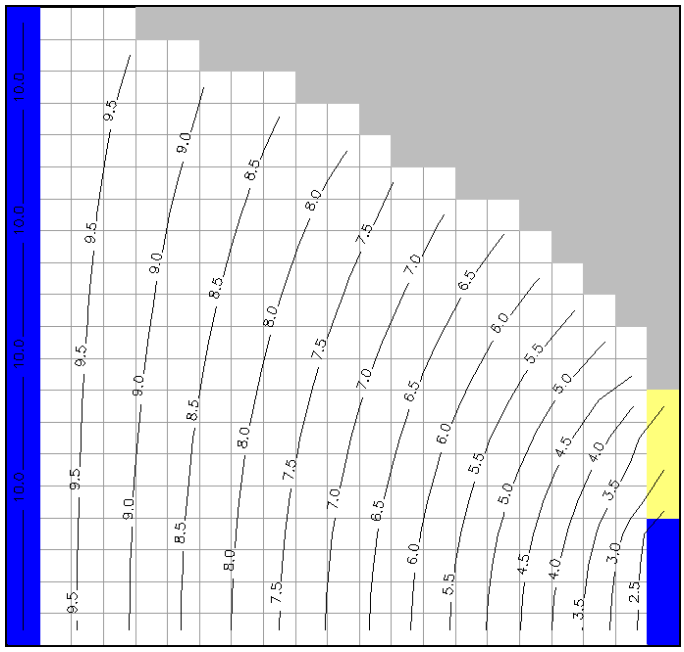


Fig. 6.52 Calculated hydraulic heads distribution and the form of the seepage surface

6.5.4 Cutoff Wall

Folder: \pm5\examples\geotechniques\geo4\

Overview of the Problem

As shown in Fig. 6.53, a highly contaminated area is located in the first stratigraphic unit of an unconfined aquifer. To the west and east of the aquifer exist fixed-head boundaries with the hydraulic head h = -0.4 m and +0.5 m. The aquifer consists of five stratigraphic units. Each unit is horizontally isotropic with uniform thickness. The elevations and horizontal hydraulic conductivities are illustrated in Fig. 6.53. The vertical hydraulic conductivities are assumed to be a tenth of the horizontal hydraulic conductivities. The effective porosity of the aquifer is 0.15. The recharge rate is 1×10^{-8} m/s.

Because of the high cost, the contaminants cannot be removed. Your task is to develop a strategy to isolate the contamination. There are four steps to be done.

1. Construct a groundwater flow model and perform a steady-state flow simulation by using the data given above and the model grid given in Fig. 6.53.
2. Geotechnical measures, such as cut-off wall, impervious cover, drain etc., can be considered as an alternative. Calculate flowlines for the case that a cut-off wall has been built to a depth of -8m and the recharge rate within the cut-off wall is reduced to zero by an impervious cover. The location of the cut-off wall is given in Fig. 6.53. When calculating the flowlines, particles should be started from the contaminated area.
3. Repeat step 3 for the case that the cut-off wall reaches the depth -10m.
4. Use a pumping well located in the cell [6, 12] to capture the contaminants. Calculate the required pumping rate and penetration depth.

Modeling Approach and Simulation Results

The aquifer is simulated using a grid of 5 layers, 23 columns and 23 rows. All layers have the same layer type **3: confined/unconfined (Transmissvity varies).** The cut-off wall is modelled by using the Horizontal-flow Barriers package. An impervious cover can be easily simulated by reducing the recharge rate. Fig. 6.54 and Fig. 6.55 show the flowlines by performing forward and backward particle tracking with PMPATH. The particles are initially placed in the center of each cell, which is located in the first model layer and within the cut-off wall. It is obvious that the contaiminants will be “washed out”, even if the cut-off wall is going deeper.

The contaminated area can be captured by using a pumping well (located in the cell [6,12])

penetrating in the first model layer with a pumping rate of 0.0025 m^3/s. This low pumping rate is possible because of the low groundwater flow velocity within the zone around the contaminated area.

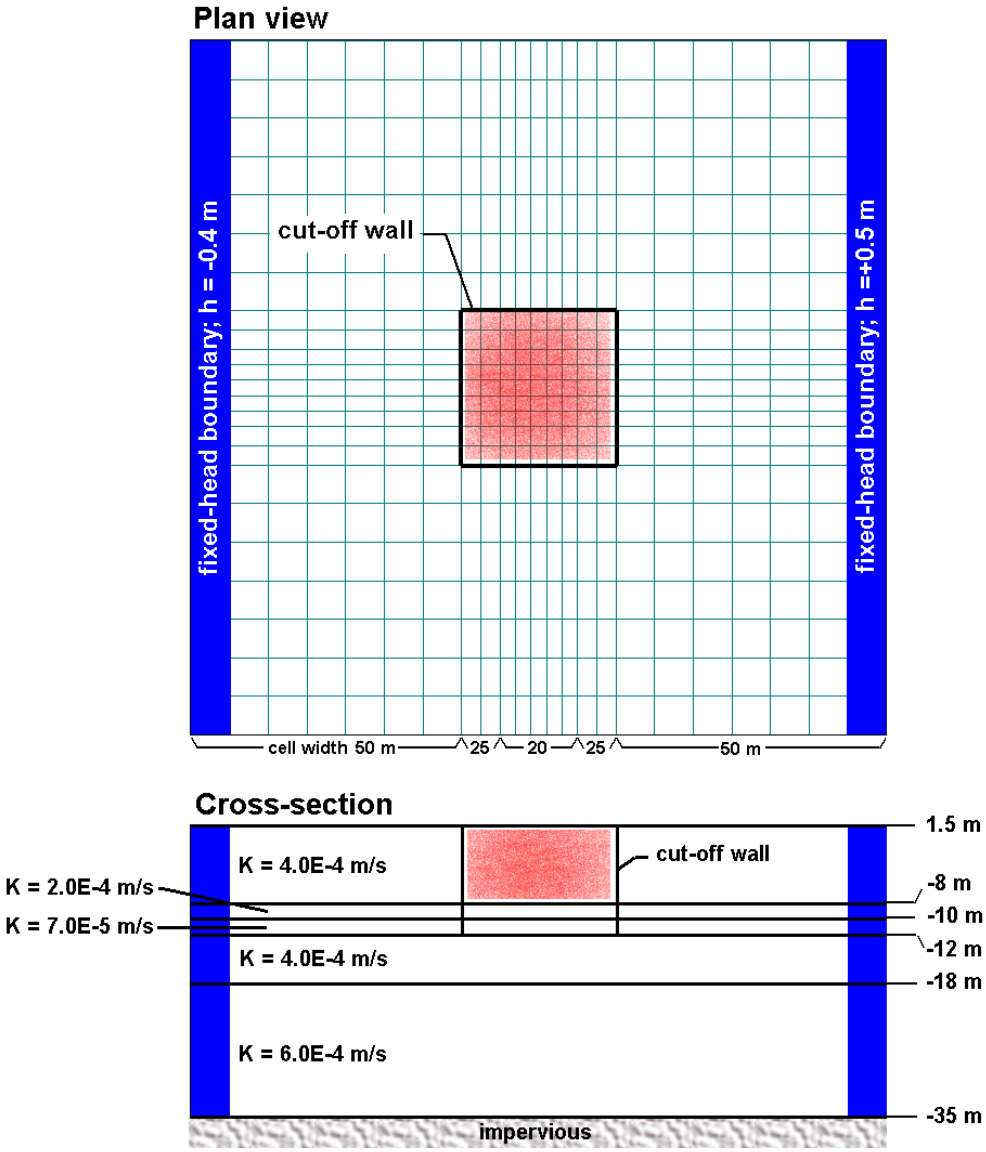


Fig. 6.53 Model grid and boundary conditions

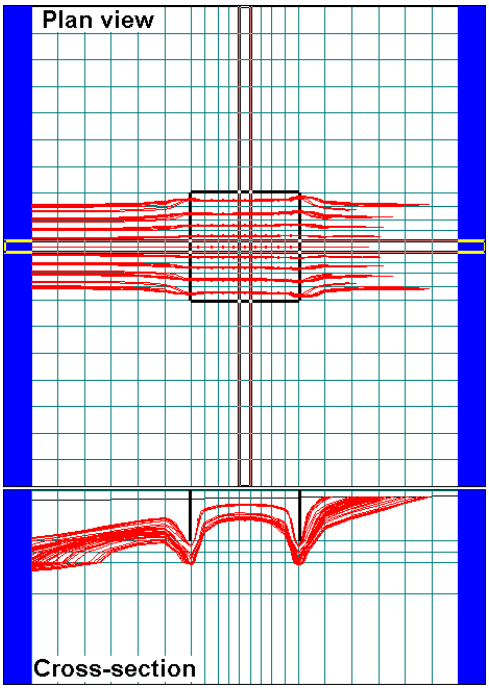


Fig. 6.54 Plan and cross-sectional views of flowlines. Particles are started from the contaminated area. The depth of the cut-off wall is -8 m.

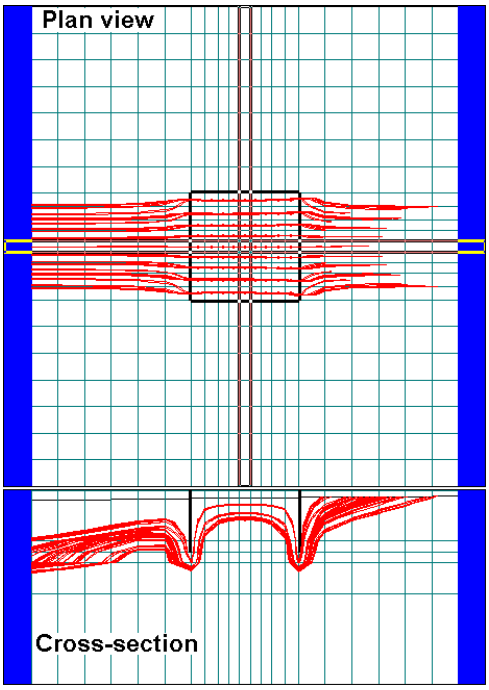


Fig. 6.55 Plan and cross-sectional views of flowlines. Particles are started from the contaminated area. The depth of the cut-off wall is -10 m.

6.5.5 Compaction and Subsidence

Folder: \pm5\examples\geotechniques\geo5\

Overview of the Problem

Fig. 6.56 shows a plan view and a cross section through an aquifer, which consists of three stratigraphic units of uniform thickness. The first unit of the aquifer is unconfined and the other units are confined. The initial hydraulic head is 43 m everywhere. The areal extent of the aquifer is assumed to be infinite large. Except a confining bed (clay) in the second unit, the sandy sediments of the aquifer are homogeneous, horizontally isotropic with an average horizontal hydraulic conductivity of 0.0001 m/s and vertical hydraulic conductivity of 0.00001 m/s. The specific yield of the first stratigraphic unit is 0.15. The specific storage of the aquifer is assumed to be 0.0001 [1/m]. The properties of the confining bed are:

horizonal hydraulic conductivity = 1×10^{-6} [m/s],
vertical hydraulic conductivity = 1×10^{-7} [m/s],
elastic specific storage = 0.002 [1/m] and
inelastic specific storage = 0.006 [1/m].

To construct a new building, an excavation pit with the size (200 m × 100 m) is required. The bottom elevation of the pit is 40 m. The pit must be held dry for one year. Your task is to calculate the required withdrawal rate and the distribution of subsidence after one year.

Modeling Approach and Simulation Results

The aquifer is simulated using a grid of 3 layers, 36 columns and 36 rows. The extent of the model grid is fairly large. Each model layer represents a stratigraphic unit. The layer type **3: confined/unconfined (Transmissvity varies)** can be used for all layers, as layers of this type switch between confined and unconfined automatically. In the **Layer Options** dialog box, the **Interbed storage** flag for the second layer is checked. The pit is modelled as fixed-head boundary with the hydraulic head h = 40 m. The compaction (and thus the land surface subsidence) of the confining bed is modelled by the Interbed Storage package.

A transient flow simulation with one stress period and 30 time steps has been carried out. The length of the stress period is one year (= 3.1536×10^7 seconds). The required withdrawal rate changes with time and can be calculated by using the water budget calculator (by assigning the zone number 1 to the pit). For the first time step, the required withdrawal rate is

0.0134 $m^3/s \approx 48.2\ m^3/h$. For the last time step, it is reduced to 0.0066 $m^3/s \approx 23.76\ m^3/h$. The distribution of the subsidence caused by this withdrawal rate can be obtained by using the **Results Extractor**. Fig. 6.57 shows the isolines of the land surface subsidence for the last time step. The maximum subsidence is about 0.11 m.

You can find two additional examples described in Leake and Prudic (1991) in the folders \...\geotechniques\geo5a\ and \...\geotechniques\geo5b\.

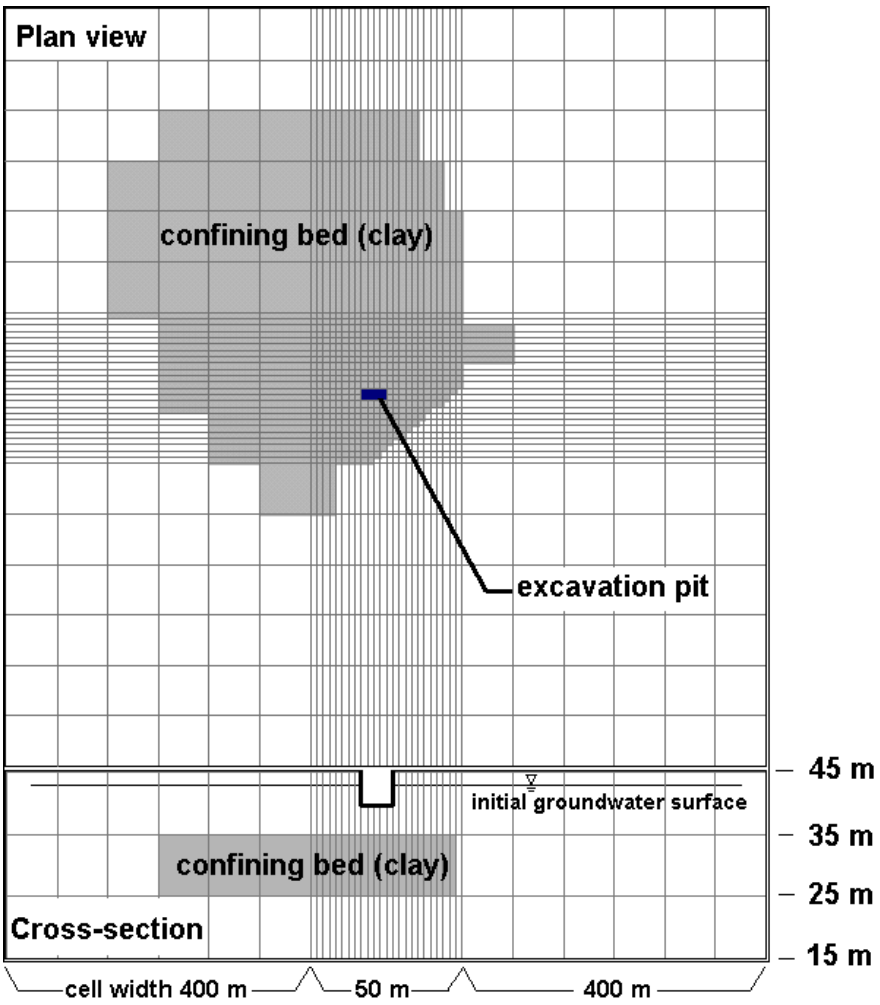


Fig. 6.56 Model grid and boundary conditions

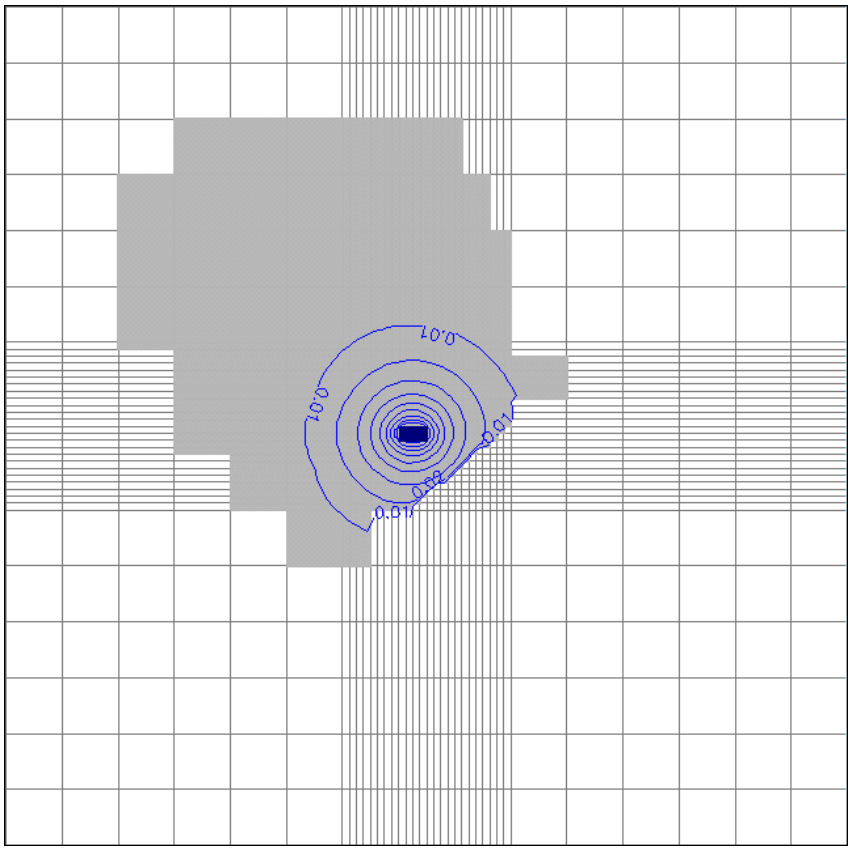


Fig. 6.57 Distribution of the land surface subsidence (maximum 0.11 m)

6.6 Solute Transport

6.6.1 One-Dimensional Dispersive Transport

Folder: \pm5\examples\transport\transport1\

Overview of the Problem

This example demonstrates the use of the numerical transport model and compares the numerical results with the analytical solution.

A uniform flow with a hydraulic gradient of 2‰ exists in a sand column. The hydraulic conductivity of the sand column is 100 m/d. The effective porosity is 0.2. The longitudinal dispersivity is 1 m. A pollutant mass of 1 g is injected into the sand column instantaneously.

Your task is to construct a one-dimensional numerical model and calculate the breakthrough curve (concentration - time curve) at 20 m downstream of the injection point. Calculate the breakthrough curve by using a longitudinal dispersivity of 4 m and compare these two curves. Will the peak arrival time of the concentration be changed if only the longitudinal dispersivity is changed?

Modeling Approach and Simulation Results

The numerical model of this example consists of one layer, one row and 51 columns. The thickness of the layer and the width of the row and column is 1 m. To obtain a hydraulic gradient of 2‰, the first cell and the last cell of the model are specifed as fixed-head cells with initial hydraulic heads of 1.1 m and 1.0 m, respectively. The initial head of all other cells is 1.0 m. A steady-state flow simulation is performed for a stress period length of 100 days.

The injected mass of 1 [g] is simulated by assigning an initial concentration of 5 [g/m^3] to the cell [10, 1, 1]. Using the **Boreholes and Observations** dialog box, an observation borehole is set in the center of the cell [30, 1, 1]. The breakthrough curves for the dispersivities of 1 m and 4 m are shown in Fig. 6.58. It is interesting to see that the concentration peak arrives earlier (with a lower concentration value) when the value of dispersivity is higher. At the first glance, this result is somewhat confusing because the center of mass should travel with the same velocity, regardless of the value of dispersivity. Because of a higher dispersivity, the front of the concentration plume travels faster and at the same time the intensity of the concentration drops faster. This combination causes this phenomenon.

Analytical solutions for solute transport involving advection, dispersion and first-order

irreversible decay in a steady-state uniform flow field are available in many text books, for example Javandel et. al (1984), Kinzelbach (1986) or Sun (1995). A computer program for the analytical solutions of 1-D and 2-D solute transport for point-like pollutant injections is provided by Rausch (1998) and included in the folder \Source\analytical solution\ of the companion CD-ROM. This program is written in BASIC and can be run by the BASIC interpreter QBASIC under MS-DOS. Try to use this program to compare the analytical and numerical solutions!

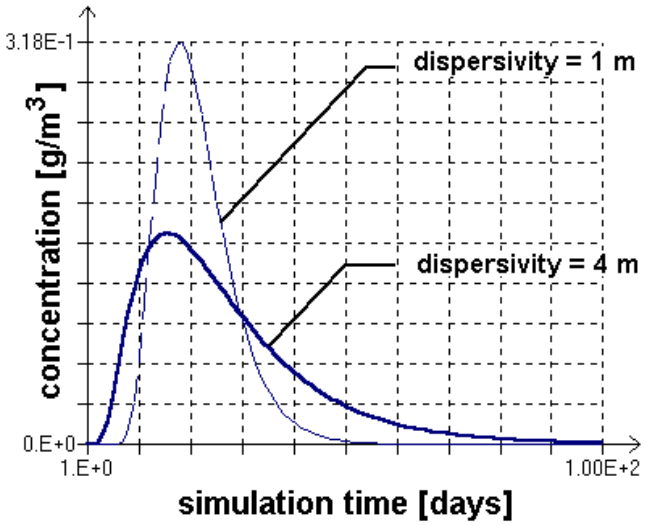


Fig. 6.58 Comparison of the calculated breakthrough curves with different dispersivity values

6.6.2 Two-Dimensional Transport in a Uniform Flow Field

Folder: \pm5\examples\transport\transport2\

Overview of the Problem

In this example, transport of solute injected continuously from a point source in a steady-state uniform flow field should be simulated. The available parameters are listed below:

Layer thickness = 10 m
Groundwater seepage velocity = l/3 m/day
Effective porosity = 0.3
Longitudinal dispersivity = 10 m
Ratio of transverse to longitudinal dispersivity = 0.3
Volumetric injection rate = 1 m^3/day
Concentration of the injected water = 1000 ppm

Your task is to construct a 2D-model and use MT3DMS to calculate the concentration distribution at the end of a 365-day simulation period.

Modeling Approach and Simulation Results

A numerical model consisting of 46 columns, 31 rows and 1 layer was constructed to simulate the problem. A regular grid spacing of 10 m is used for each column and row. The configuration of the model is shown in Fig. 6.59. The model layer is simulated as a confined layer. The top and bottom of the model layer are at an elevation of 10 m and 0 m, respectively. To simulate the groundwater seepage velocity of 1/3 m/day, fixed-head boundaries (with h = 11 m and h = 10 m) are assigned to the west and east side of the model. The horizontal hydraulic conductivity is 45 m/day.

The flow field was first calculcated by MODFLOW. The third order TVD scheme was used in the simulation for the advection term; and the GCG solver is used to solve the system equations. The contour map of the concentration field at the end of the 365-day simulation period obtained for this example is shown in Fig. 6.60. An analytical solution for this problem is given by Wilson and Miller (1978). The analytical solution is applicable only under the assumption that 1) the aquifer is relatively thin, so that instantaneous vertical mixing can be assumed; 2) the injection rate is insignificant compared with the ambient uniform flow.

Fig. 6.61 shows the breakthrough curves at an observation well located 60 m downstream of the injection well. The analytical solution is obtained by using the computer program (Rausch,

1998) included in the folder \Source\analytical solution\ of the companion CD-ROM. Fig. 6.62 compares the analytical solution with the numerical solution obtained by using the upstream finite difference method. The numerical dispersion is significant when the upstream finite difference method is used to solve the advection term.

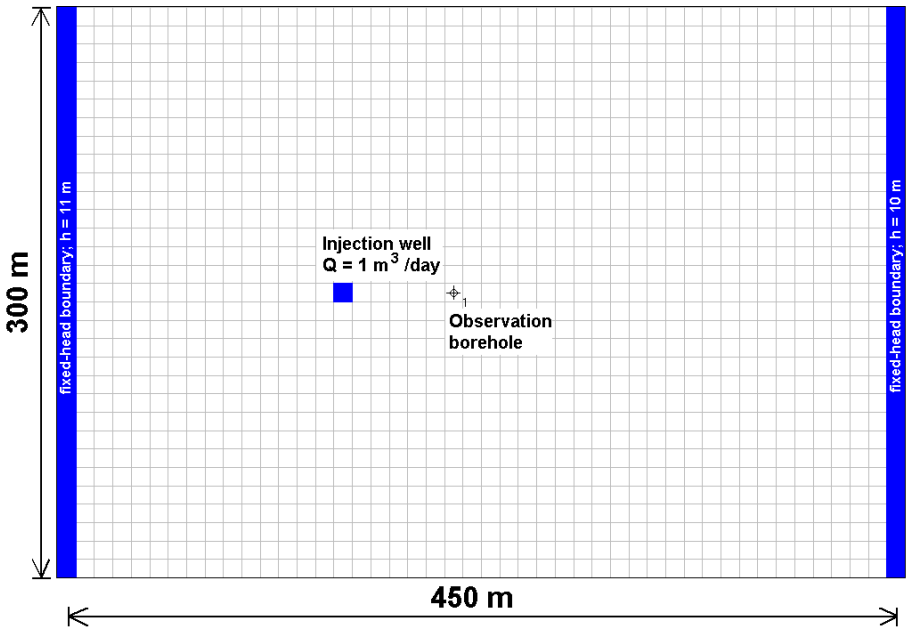


Fig. 6.59 Configuration of the model and the location of an observation borehole

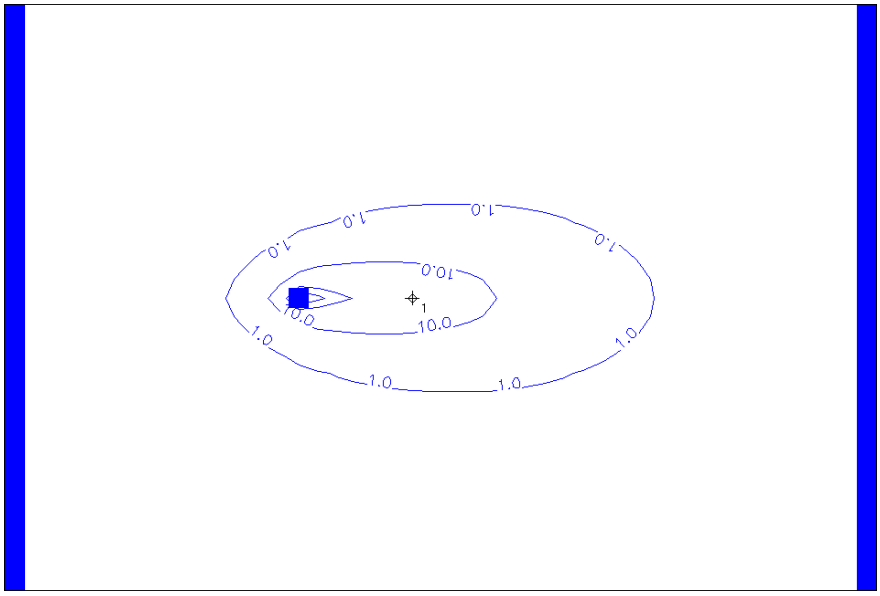


Fig. 6.60 Calculated concentration distribution

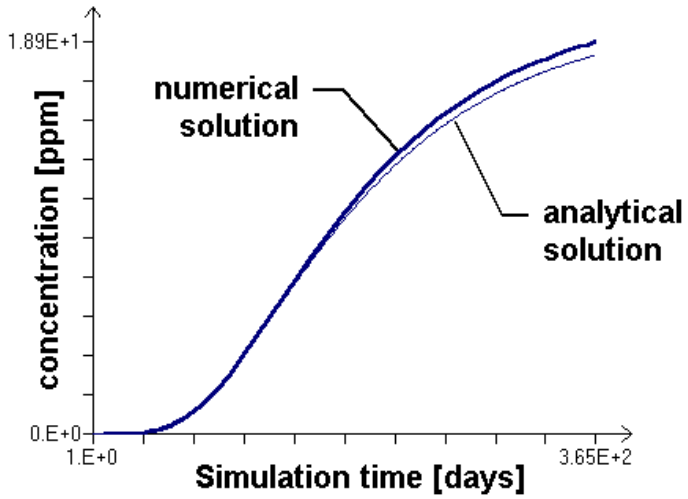


Fig. 6.61 Comparison of the breakthrough curves at the observation borehole. The numerical solution is obtained by using the 3rd order TVD scheme.

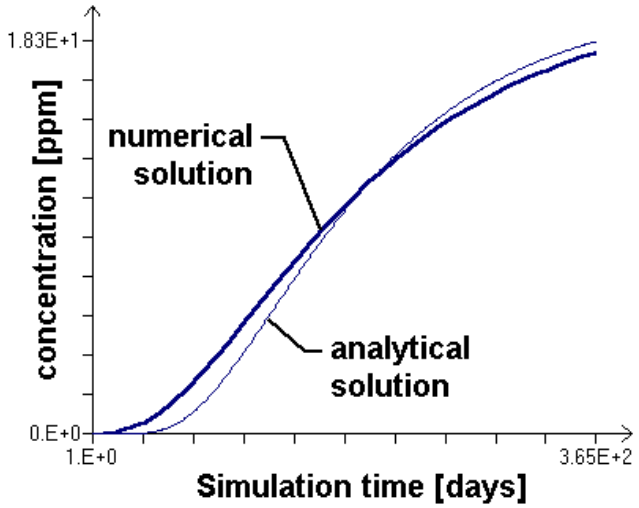


Fig. 6.62 Comparison of the breakthrough curves at the observation borehole. The numerical solution is obtained by using the upstream finite difference method.

6.6.3 Benchmark Problems and Application Examples from Literature

Folder: \pm5\examples\transport\

Overview of the Problems

To test the accuracy and performance of the MT3D/MT3DMS and MOC3D codes, several benchmark problems and application examples are introduced in the user's guides of MT3D (Zheng, 1990), MT3DMS (Zheng and Wang, 1998) and MOC3D (Konikow et al., 1998). You can find these documentations on the folders \document\mt3d\, \document\mt3dms\ and \document\moc3d\ of the companion CD-ROM. Either analytical solutions or numerical solutions by another code can serve as benchmark problems.

Modeling Approach and Simulation Results

Using PMWIN we have rebuilt most of the benchmark problems of MT3D/MT3DMS and MOC3D. If you have selected to install the component *Solute transport* during the installation of PMWIN, you can find the models in the sub-folders under \PM5\examples\Transport\ listed in Table 6.7. All these models are ready-to-run. It is recommended that the users try these test problems first to become familiarized with the various options before applying MT3D/MT3DMS or MOC3D to solve their own problems.

Table 6.7 Benchmark problems and application examples of MT3D/MT3DMS and MOC3D

Folder	Description
\PM5\...\TRANSPORT3\	This model is described in section 7.5 of the manual of MT3DMS. A numerical model consisting of 31 columns, 31 rows and 1 layer is used to simulate the two-dimensional transport in a radial flow field; numerical results were compared with the analytical solution of Moench and Ogata (1981).
\PM5\...\TRANSPORT4\	This model is described in section 7.6 of the manual of MT3DMS. A numerical model consisting of 31 columns, 31 rows and 1 layer is used to simulate the concentration change at the injection/extration well; numerical results were compared with the approximate analytical solution of Gelhar and Collins (1971).
\PM5\...\TRANSPORT5\	This model is described in section 7.7 of the manual of MT3DMS. A numerical model consisting of 21 columns, 15 rows and 8 layers is used to solve three-dimensional transport in a uniform flow field. The point source was simulated at column 3, row 8 and layer 7. Numerical results were compared with the analytical solution of Hunt (1978).
\PM5\...\TRANSPORT6\	This model is described in section 7.9 of the manual of MT3DMS. This example illustrates the application of MODFLOW and MT3D/MT3DMS to a problem involving transport of contaminants in a two-dimensional heterogeneous aquifer.

Table 6.7 (continued)

\PM5\...\TRANSPORT7\	This model is described in section 7.10 of the manual of MT3DMS. This example illustrates the application of MT3D/MT3DMS to an actual field problem involving the evaluation of the effectiveness of proposed groundwater remediation schemes.
\PM5\...\TRANSPORT8\	This model is described in the section *MODEL TESTING AND EVALUATION - One-Dimensional Steady Flow* of the user's guide of MOC3D. A numerical model consisting of 122 columns, 1 row and 1 layer is used to simulate one-dimensional transport having a third-type source boundary condition in a steady-state flow field; numerical results were compared with the analytical solution of Wexler (1992).
\PM5\...\TRANSPORT9\	This model is described in the section *MODEL TESTING AND EVALUATION - Three-Dimensional Steady Flow* of the user's guide of MOC3D. A numerical model consisting of 12 columns, 32 rows and 40 layers is used to simulate three-dimensional transport having a permanent point source in a steady-state flow field; numerical results were compared with the analytical solution of Wexler (1992).
\PM5\...\TRANSPORT10\	This model is described in the section *MODEL TESTING AND EVALUATION - Two-Dimensional Radial Flow and Dispersion* of the user's guide of MOC3D. A numerical model consisting of 30 columns, 30 rows and 1 layer is used to simulate two-dimensional transport having a permanent point source in a steady-state radial flow field; numerical results were compared with the analytical solution given by Hsieh (1986).
\PM5\...\TRANSPORT11\	This model is described in the section *MODEL TESTING AND EVALUATION - Point Initial Condition in Uniform Flow* of the user's guide of MOC3D. A numerical model consisting of 26 columns, 26 rows and 26 layer is used to simulate three-dimensional transport having an initial point source in a parallel steady-state flow at 45 degrees to the x-direction; numerical results were compared with the analytical solution given by Wexler (1992). The point source was simulated at column 4, row 4 and layer 12.

6.7 Miscellaneous Topics

6.7.1 Using the Field Interpolator

Folder: \pm5\examples\misc\misc1\

Overview of the Problem

This example illustrates the use of the Field Interpolator. Fig. 6.63 shows the plan view of the model area, the model grid and the locations of measurement points. The model grid consists of 70 rows, 60 columns, and one layer. The measured hydraulic heads and the coordinates of the measurement points are saved in the file \pm5\examples\misc\misc1\measure.dat. To obtain the starting head distribution of a flow simulation, the measured hydraulic heads should be interpolated to each model cell.

Modeling Approach and Simulation Results

The starting heads are interpolated to model cells using the four interpolation methods provided by the Field Interpolator. The interpolation results are shown in the form of contours in Fig. 6.64 - 6.67. The **octant** search method with **Data Per Sector** = 1 is used by all gridding methods. A weighting exponent of $F = 2$ is used by Shepard's inverse distance method. The Kriging method uses the linear variogram model with $c_0 = 0$ and $\alpha = 1$. There is no significant difference observed in these figures when sufficient data points are available. The major difference is observed in the southern part of the model area, where only one measurement point is found and the system is not well conditioned.

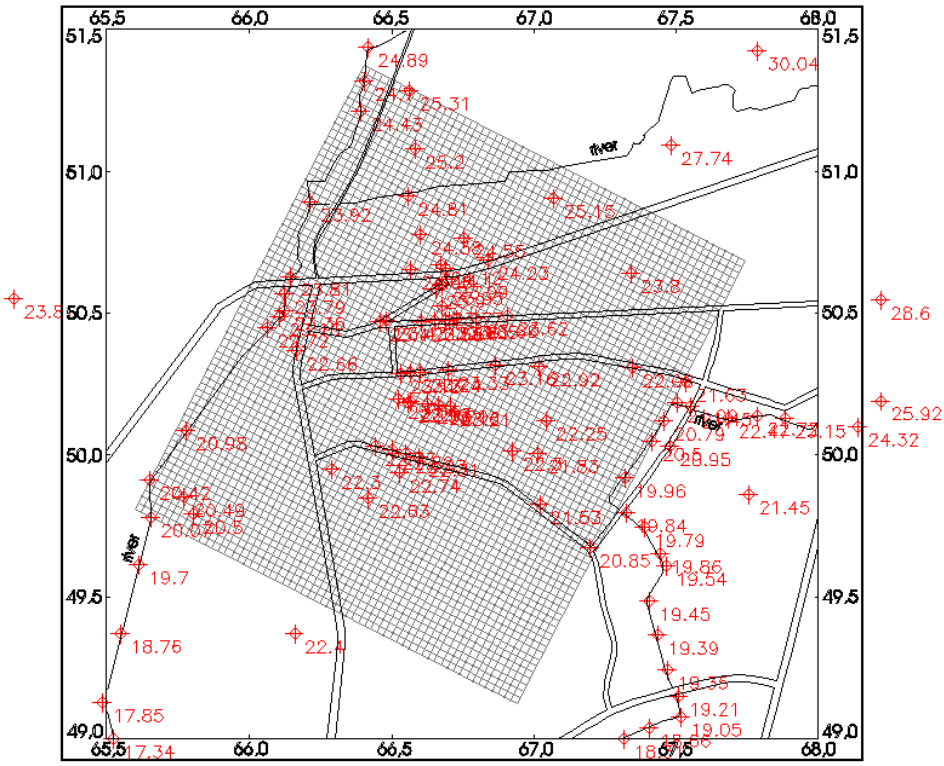


Fig. 6.63 Model domain and the measured hydraulic heads

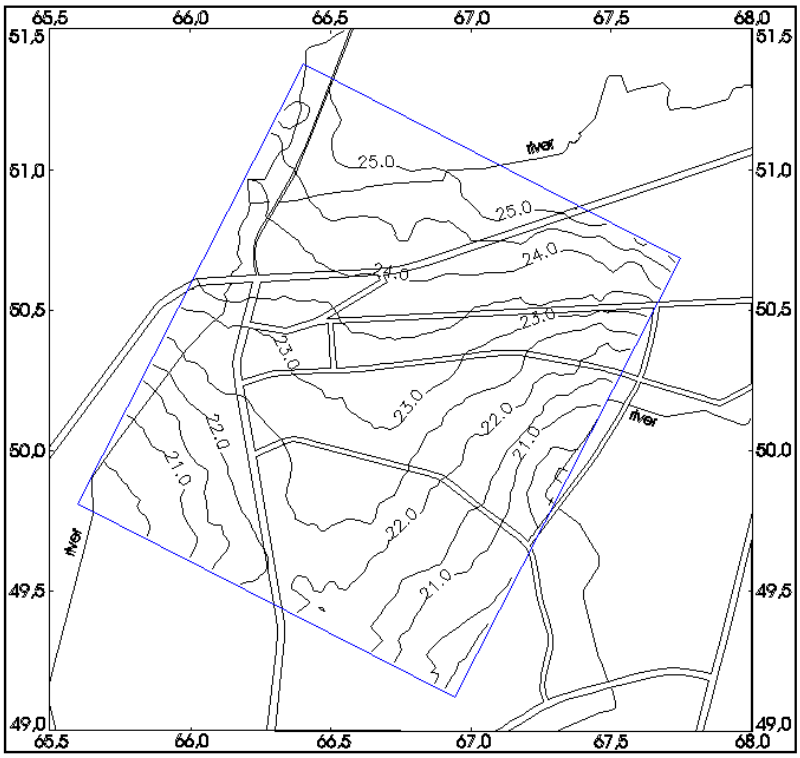


Fig. 6.64 Contours produced by Shepard's inverse distance method

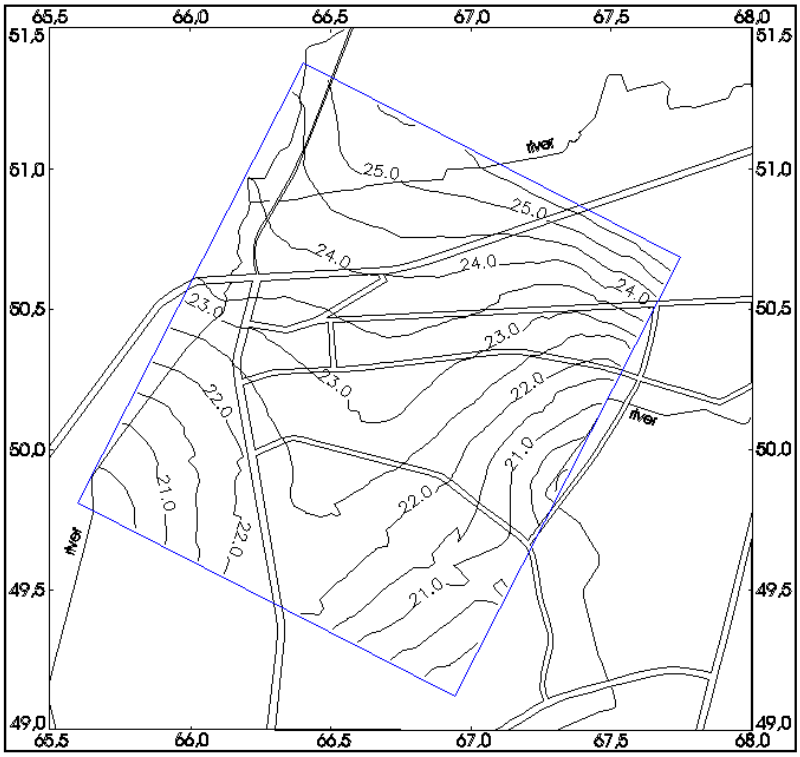


Fig. 6.65 Contours produced by the Kriging method

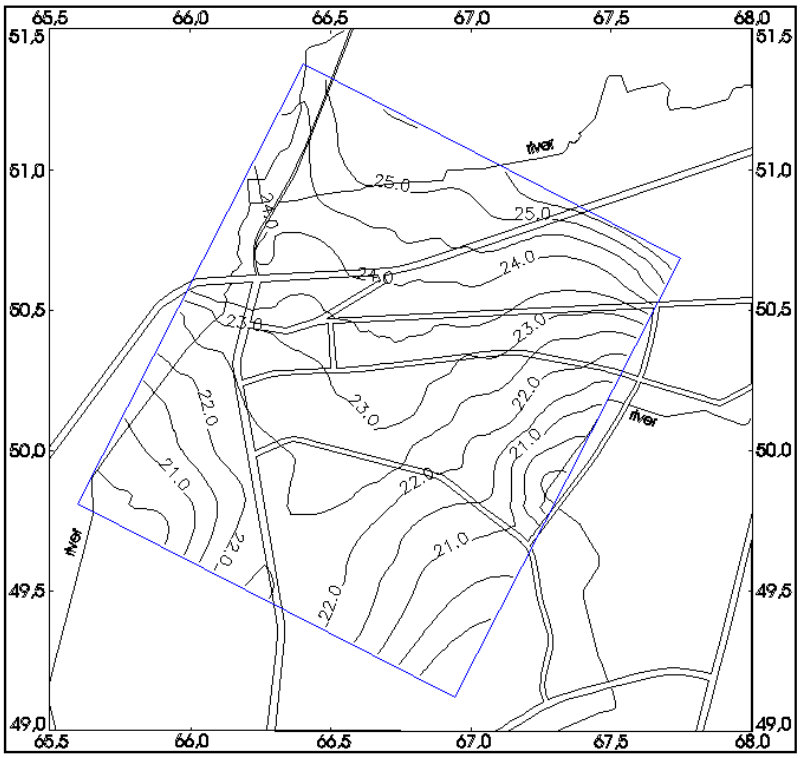


Fig. 6.66 Contours produced by Akima's bivariate interpolation

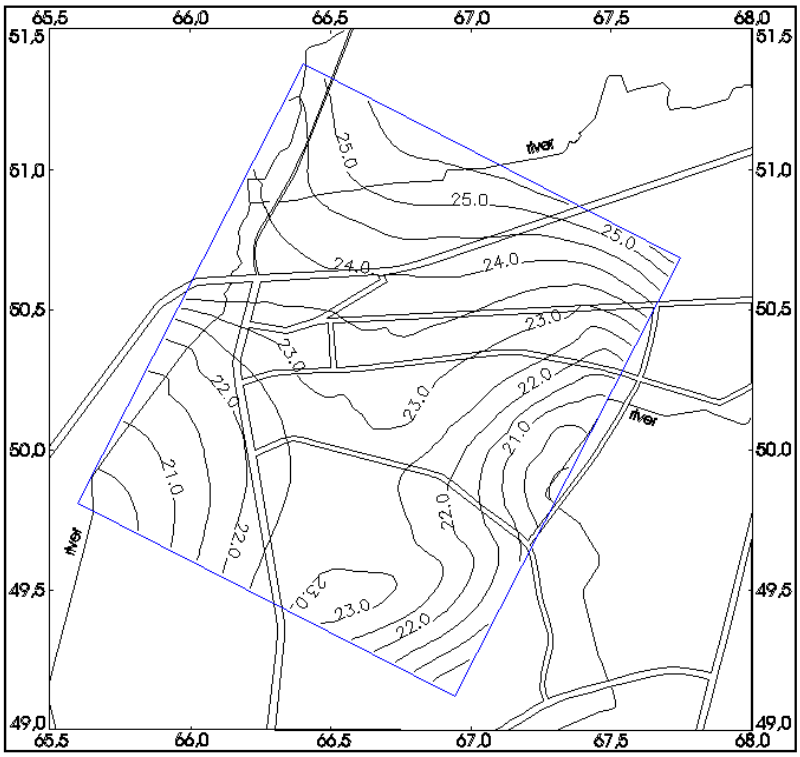


Fig. 6.67 Contours produced by Renka's triangulation algorithm

6.7.2 An Example of Stochastic Modeling

Folder: \pm5\examples\misc\misc2\

Overview of the Problem

Aquifer remediation measures are often designed by means of groundwater models. Model results are usually uncertain due to the imperfect knowledge of aquifer parameters. We are uncertain about whether the calibrated values of parameters represent the real aquifer system. We never know the actual small-scale distribution of some parameters, e.g. hydraulic conductivity or recharge. Thus, all groundwater models involve uncertainty. Stochastic models are often employed to take into account uncertainty. In the stochastic modeling approach, the model parameters appear in the form of probability distributions of values, rather than as deterministic sets.

We use the aquifer described in chapter 2 to illustrate the concept of stochastic modeling. Using a two-dimensional approach to model the aquifer, we may utilize the **Field Generator** to create lognormal correlated distributions of the horizontal hydraulic conductivity. The mean horizontal hydraulic conductivity of the aquifer is equal to $(4 \times 0.0001 + 6 \times 0.0005) / 10 = 3.4 \times 10^{-4}$ m/s. The standard deviation is assumed to be $F = 0.5$. A correlation length of 60 m is used.

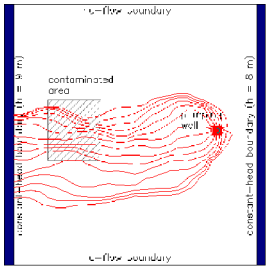
In chapter 2, the pumping rate of the well was determined such that the contaminated area lies within the capture zone of the well. When different realizations of the heterogeneous distribution of hydraulic conductivity are introduced, it is obvious that the capture zone not always covers the entire contaminated area. The safety criterion for the measure can be defined as the percentage of the covered area in relation to the entire contaminated area. The expected value of the safety criterion can be obtained from stochastic simulation.

Modeling Approach and Simulation Results

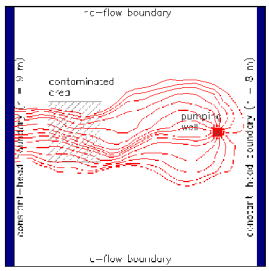
Using the **Field Generator,** lognormal distributions of the horizontal hydraulic conductivity are generated and stored in ASCII Matrix files. First, each generated realization is imported into the horizontal hydraulic conductivity matrix, then a flow simulation is performed. The capture zone of the pumping well, as well as pathlines, are computed with PMPATH. The resulting safety criterion is obtained by a Monte Carlo simulation. This implies that many realizations of the parameter field are produced and used in the flow simulation.

Fig. 6.68 shows results of five realizations and the calculated mean safety criterion. The

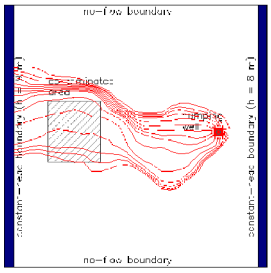
mean safety criterion is the sum of safety criteria divided by the number of realizations. A large number of realizations may be required for the mean safety criterion to converge.



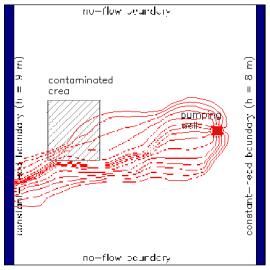
Realization 1
Safety Criterion = 85 %
Mean Safety Criterion = 85%



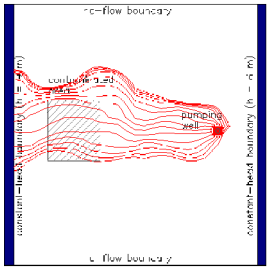
Realization 2
Safety Criterion = 87 %
Mean Safety Criterion = 86%



Realization 3
Safety Criterion = 97 %
Mean Safety Criterion = 89.7%



Realization 4
Safety Criterion = 48 %
Mean Safety Criterion = 79.3%



Realization 5
Safety Criterion = 93 %
Mean Safety Criterion = 82%

Fig. 6.68 Calculation of the mean safety criterion by the Monte Carlo method

FOR YOUR NOTES

7. Appendices

Appendix 1: Limitation of PMWIN

This section gives the size limitation of PMWIN. Refer to the documentation of individual packages for their assumptions, applicability and limitations.

Data Editor

Maximum number of layers = 80
Maximum number of stress periods = 1000
Maximum number of cells along rows or columns = 2000
Maximum number of cells in a layer = 250000
Maximum number of zones in a layer = 20
Maximum number of vertex nodes of a zone = 40
Maximum number of stream segments = 25
Maximum number of tributary segments of each stream segment = 10
Maximum number of reservoirs = 20
Maxmum number of observated stages of each reservoir = 200

There is no limit to the number of wells, general-head boundary cells, rivers, drains and horizontal-flow-barrier cells.

Boreholes and Observations

Maximum number of boreholes = 1000
Maximum number of observations = 10000

Digitizer

Maximum number of digitized points 10000

Field Interpolator

Maximum number of cells in a layer = 250000
Maximum number of cells along rows or columns = 2000
Maximum number of input data points = 2000

Field Generator

Maximum number of cells in a layer = 250000
Maximum number of cells along rows or columns = 500

Water Budget Calculator

Maximum number of subregions = 50

Appendix 2: Files and Formats

ASCII Matrix File

An ASCII Matrix file can be saved or loaded by the **Browse Matrix** dialog box (see section 3.8). The Results Extractor, Field Interpolator and Field Generator use this file format to save the generated data.

File Format

1. Data: NCOL NROW
2. Data: MATRIX (NCOL, NROW)

Explanation of Fields Used in Input Instructions

ALL DATA IN THE SAME RECORD ARE SEPARATED BY A COMMA OR BLANK.

NCOL	is the number of model columns.
NROW	is the number of model rows.
MATRIX	is a two dimensional data matrix saved row by row. Matrix can be saved in free format. If the wrap from is used to save the matrix, each line of the matrix contains up to 20 values.

Example

If NCOL=6 and NROW=5, an ASCII Matrix file would be

```
6  5
121  152  133  144  315  516
221  252  233  244  215  216
321  352  333  344  315  316
421  452  433  444  415  416
521  552  533  544  515  516
```

Or

```
6  5
121  152  133  144  315  516  221  252  233  244  215  216
321  352  333  344  315  316  421  452  433  444  415  416
521  552  533  544  515  516
```

Boreholes file

A borehole file can be saved or loaded by the **Boreholes and Observations** dialog box (see section 3.5).

File Format

1. Data: LABEL
2. Data: NB XXX XXX XXX XXX

(The following data repeats NB times)

3. Data: ACTIVE X Y LAYER DRAW COLOR NAME

Explanation of Fields Used in Input Instructions

ALL DATA IN THE SAME RECORD ARE SEPARATED BY A COMMA OR BLANK.

LABEL	is the file label. It must be **PMWIN5000_BOR_FILE**
NB	is the number of boreholes. Maximum number of NB is 1000.
XXX	reserved.
ACTIVE	A borehole is active, if Active = 1.
X	is the x-coordinate of the borehole.
Y	is the y-coordinate of the borehole.
LAYER	is the layer number of the borehole.
DRAW	If DRAW = -1, the obervation vs. time curve of a borehole will be shown when the Graphs Viewer is activated.

COLOR is the color used to draw the obervation vs. time curve of a borehole. The color is defined by a long integer using the equation: color = red + green × 256 + blue × 65536, where red, green and blue are the color components ranging from 0 to 255.
NAME is the name of the borehole.

Contour Table file

A contour table file can be saved or loaded by the Environment dialog box (see section 3.8).

File Format

1. Data: LABEL
2. Data: NL XXX XXX XXX XXX

(The following data repeats NB times)

3. Data: LEVEL COLOR FILL LVISIBLE LSIZE LDIS XXX XXX XXX

Explanation of Fields Used in Input Instructions

ALL DATA IN THE SAME RECORD ARE SEPARATED BY A COMMA OR BLANK.

LABEL is the file label. It must be **PMWIN5000_CONTOUR_FILE**
NL is the number of contour levels
XXX reserved.
LEVEL Contour level
COLOR is the color used to draw the contour line; The color is defined by a long integer using the equation: color = red + green × 256 + blue × 65536, where red, green and blue are the color components ranging from 0 to 255.
FILL is the color used to fill the space between the current contour and the next contour level.
LVISIBLE the contour is visible if LVISIBLE is TRUE.
LSIZE is the appearance height of the label text in the same unit as the model.
LDIS is the the distance between two contour labels, in the same unit as the model.

Grid Specification File

The grid specification file provides the grid geometry and location details.

File Format

1. Data: NROW NCOL
2. Data: X Y ANGLE
3. Data: DELR(NCOL)
4. Data: DELC(NROW)
5. Date: X1, Y1
6. Data: X2, Y2
7. Data: NLAY

Explanation of Fields Used in Input Instructions

NROW is the number of model rows.
NCOL is the number of model columns.
X is the x-coordinate of the top-left corner of the model grid.
Y is the y-coordinate of the top-left corner of the model grid.
ANGLE is the rotation angle expressed in degrees and measured countercolckwise from the positive x-axis.
DELR is the cell width along rows. Read one value for each of the NCOL columns. This is a single array with one value for each column.
DELC is the cell width along columns. Read one value for each of the NROW rows. This is a single array with one value for each row.
X1, Y1 is the coordinates of the lower-left corner of the model worksheet (see Coordinate System for details).

X2, Y2 is the coordinates of the upper-right corner of the model worksheet (see Coordinate System for details).
NLAY is the number of model layers.

Line Map file

A line map file contains a series of polylines, each polyline is defined by the number of vertices and a series of coordinate pairs.

File Format

Repeat Data 1 and 2 for each polyline
1. Data: NVERTEX

(The following data repeats NVERTEX times)
2. Data: X Y

Explanation of Fields Used in Input Instructions

ALL DATA IN THE SAME RECORD ARE SEPARATED BY A COMMA OR BLANK.
NVERTEX is the number of vertices of a polyline
X is the x-coordinate of the i-th vertex
Y is the y-coordinate of the i-th vertex

Observation File

An observation file can be created by the **Boreholes and Observations** dialog box (see section 3.5) or the Graphs Viewer (see section 5.6). An existing observation file can be imported into the **Boreholes and Observations** dialog box.

File Format

1. Data: LABEL
2. Data: NOBS XXX XXX XXX XXX

(The following data repeats NOBS times)
3. Data: TIME WEIGHT HEAD DDOWN CONC COMPAC PREHEAD SUBSDNS NAME

Explanation of Fields Used in Input Instructions

ALL DATA IN THE SAME RECORD ARE SEPARATED BY A COMMA OR BLANK.
LABEL is the file label. It must be PMWIN5000_OBS_FILE
NOBS is the number of observations. Maximum number of NOBS is 10000.
XXX reserved.
BORENO is the borehole number where the observation is made.
TIME is the observation time, measured from the start of the simulation.
WEIGHT is the weight attached to each observation
HEAD is the observed head at time TIME.
DDOWN is the observed drawdown at time TIME.
CONC is the observed concentration at time TIME.
COMPAC is the compaction at time TIME
PREHEAD is the preconsolidation head at time TIME.
SUBSDNS is the subsidence at time TIME.
NAME is the name of the borehole at which the observations are made.

Time Parameter File

A Time Parameter file can be saved or loaded by the Time Parameter dialog box (see section 3.3.3).

File Format

1. Data: NPER ITMUNI

(The following data repeats NPER times)
2. Data: ACTIVE PERLEN NSTP TSMULT DT0 MXSTRN TTSMULT

Explanation of Fields Used in Input Instructions

ALL DATA IN THE SAME RECORD ARE SEPARATED BY A COMMA OR BLANK.

NPER	is the number of stress periods in the simulation
ITMUNI	indicates the time unit of model data. (It is used only for printout of elapsed simulation time. It does not affect model calculations.) 0 - undefined 1 - seconds 2 - minutes 3 - hours 4 - days 5 - years The unit of time must be consistent for all data values that involve time. For example, if years is the chosen time unit, stress-period length, timestep length, transmissivity, etc., must all be expressed using years for their time units. Likewise, the length unit must also be consistent.
ACTIVE	A stress period is active, if ACTIVE = -1. Set ACTIVE=0, if a stress period is inactive.
PERLEN	is the length of a stress period. It is specified for each stress period.
NSTP	is the number of time steps in a stress period.
TSMULT	is the multiplier for the length of successive time steps. The length of the first time step DELT(1) is related to PERLEN, NSTP and TSMULT by the relation DELT(1) = PERLEN(1-TSMULT)/(1-TSMULT**NSTP).
DT0	is the length of transport steps. If DT0=0, the length of transport steps will be determined by an automatic stepsize control procedure in MT3D.
MXSTRN	is the maximum number of transport steps.
TTSMULT	is the multiplier for the length of successive transport steps within a flow time step, if the Generalized Conjugate Gradient (GCG) solver is used and the solution option for the advection term is the upstream finite difference method.

Trace File

A Trace file can be saved or loaded by the Search and Modify dialog box (see section 3.3.7).

File Format

1. Data: LABEL

(The following data repeats 50 times, one record for each search range)
3. Data: ACTIVE COLOR MIN MAX VALUE OPTION

Explanation of Fields Used in Input Instructions

ALL DATA IN THE SAME RECORD ARE SEPARATED BY A COMMA OR BLANK.

LABEL	is the file label. It must be PMWIN4000_TRACEFILE
ACTIVE	a search range (see MIN / MAX below) is active, if ACTIVE = -1
COLOR	is the fill color. The color is defined by a long integer using the equation: color = red + green × 256 + blue × 65536, where red, green and blue are the color components ranging from 0 to 255. COLOR is assigned to the finite-difference cells that have a value located within the search range (see MIN / MAX below).
MIN / MAX	define the lower limit and upper limit of the search range.
VALUE	According to OPTION (see below), you can easily modify the cell values (see section 3.3.7 for details.)
OPTION	OPTION = 0, Display only. OPTION = 1, Replace: The cell values are replaced by VALUE. OPTION = 2, Add: VALUE is added to the cell values. OPTIOn = 3, Multiply: The cell values are multiplied by VALUE.

Zone file

A zone file can be saved or loaded by the Data Editor by using the item Zones from the Value menu.

File Format

1. Data: LABEL
2. Data: NZONES, XXX, XXX, XXX, XXX

(The following data (data 3-6) repeat NZONES times)

3. Data: NP
4. Data: PARNO
5. Data: Value(1) Value(2) Value(3) ... Value(I) ... Value(16)

(The following data repeats NP times)

6. Data: X(J), Y(J)

Explanation of Fields Used in Input Instructions

ALL DATA IN THE SAME RECORD ARE SEPARATED BY A COMMA OR BLANK.

LABEL is the file label. It must be PMWIN4000_ASCII_ZONEFILE

NZONES is the number of zones. Maximum is 20.

XXX reserved.

NP is the number of nodes of each zone. The first and the last node must overlap. The maximum number of NP is 41.

PARNO is the assigned parameter number (see section 3.3.6 for how to define an estimated paramter)

Value(I) I = 1 to 16; Value(I) are the zone values. For aquifer parameters, such as porosity or transmissivity, only the first value (or two values, if a parameter number can be defined) is used. For MODFLOW packages, such as Drain Package, as many values as required by the package are used. For example, two values (Hydraulic conductance and the elevation of the drain) required for defining a drain will be saved in Value(1) and Value(2). Other values that are not used must be specified as zero. The following table gives the assignment of the parameters in the Value(I) vector. Refer to section 3.6.1 for the definitions of the parameters.

Package	Value(1)	Value(2)	Value(3)	Value(4)
WEL1	Recharge rate	XXX	XXX	XXX
DRN1	Hydr. conductance	Elevation	XXX	XXX
RIV1	Hydr. conductance	Head in river	Elevation	XXX
EVT1	Max. ET rate	ET Surface	Extinction Depth	Layer Indicator
GHB1	Hydr. conductance	Head at boundary	XXX	XXX
RCH1	Recharge Flux	Layer Indicator	XXX	XXX
HFB1	Barrier Direction	K/Thickness	XXX	XXX
IBS1	Preconlidation head	Elastic storage	Inelastic storage	Starting compaction
CHD1	Flag	Start head	End head	XXX

The values used by the STR1 package are
Value(1) = Segment; Value(2) = Reach; Value(3) = StreamFlow; Value(4) = Stream stage;
Value(5) = Hydr. conductance; Value(6) = Elavation of the streambed top;
Value(7) = Elavation of the streambed bottom; Value(8) = Stream width;
Value(9) = Stream slope; Value(10) = Manning's roughness coefficient divided by C.

X(J),Y(J) are the (x,y) coordinates of the J-th node of the zone. The first and the last node must overlap.

Appendix 3: Input Data Files of the supported Models

The following tables gives the name of input data files for each packages of the supported models. The input files are saved in the same folder as the model data. Refer to the documentation of corresponding models for the format of the input files. You can find the documentions in the folder \document\ of the companion CD-ROM.

Name File

MODFLOW-88, MODFLOW-96 and MOC3D require a so-called **Name File**. The name file is also required if you want to import an existing model into PMWIN. The name file contains a list of file types, unit numbers and the associated file name.

File Format

1. Data: FTYPE NUNIT FNAME

Explanation of Fields Used in Input Instructions

ALL DATA IN THE SAME RECORD ARE SEPARATED BY A COMMA OR BLANK.

FTYPE iis the file type, which must be one of the following character values. FTYPE may be entered in uppercase or lowercase.

- LIST for the simulation listing file
- BAS for the Basic Package
- OC for the Output Control Option
- BCF for the Block-Centered Flow Package
- RCH for the Recharge Package
- RIV for the River Package
- WEL for the Well Package
- DRN for the Drain Package
- GHB for the General-Head Boundary Package
- EVT for the Evapotranspiration Package
- SIP for the Strongly Implicit Procedure Package
- SOR for the Slice-Successive Over-Relaxation Package
- DATA(BINARY) for binary (unformatted) files such as those used to save cell-by-cell budget data and binary (unformatted) head and drawdown data.
- DATA for formatted (text) files such as those used to save formatted head and drawdown and for input of array data from files that are separate from the primary package input files.

NUNIT is the Fortran unit to be used when reading from or writing to the file. Any legal unit number on the computer being used can be specified except units 97-99. Unit 99 is used for the name file and for reading arrays using the OPEN/CLOSE option (see Input Instructions for Array Reading Utility Modules section). Units 97 and 98 are used for batch files as explained below. Each file must have a unique unit number.

FNAME is the name of the file, which is a character value.

Notes:

1. **If you want to import a model into PMWIN, all files listed in the Name File must be located in the same folder as the Name File itself.**
2. **Although MODFLOW allows array values of some packages (BAS, BCF, EVT and RCH) to be saved in extra data files by using DATA(BINARY) or DATA, these features are not supported by the converter of PMWIN. You must put the external array values into the package files before converting the model.**
3. **An imported model will have the same model name as the Name File.**

Example of a Name File

This example file is generated by PMWIN for the model located in \pm5\examples\basic\basic1\. The file name is basic1.nam.

```
LIST        6    output.dat
BAS         1    bas.dat
BCF         11   bcf.dat
OC          22   oc.dat
```

WEL	12	wel.dat
RCH	18	rch.dat
PCG	23	pcg2.dat
DATA(BINARY)	50	budget.dat
DATA(BINARY)	51	heads.dat
DATA(BINARY)	52	ddown.dat
DATA(BINARY)	32	mt3d.flo

MODFLOW

Basic Package . . . . . BAS.DAT
Block-Centered Flow Package . . . . . BCF.DAT
Density Package (DEN1) DEN1.DAT
Direct Solution Package (DE45) DE45.DAT
Drain Package . . . . . DRN.DAT
Evapotranspiration Package . . . . . EVT.DAT
General-Head Boundary Package . . . . . GHB.DAT
Horizontal-Flow Barrier Package HFB1.DAT
Interbed-Storage Package IBS1.DAT
Output Control . . . . . OC.DAT
Preconditioned Conjugate Gradient 2 Package (PCG2) PCG2.DAT
River Package . . . . . RIV.DAT
Recharge Package . . . . . RCH.DAT
Reservoir Package RES1.DAT
Strongly Implicit Procedure Package . . . . . SIP.DAT
Slice-Successive Overrelaxation Package . . . . . SOR.DAT
Stream-Routing Flow Package STR1.DAT
Time-Variant Specified-Head CHD1.DAT
Well Package . . . . . WEL.DAT

MODPATH and MODPATH-PLOT (version 1.x)

Main data file . . . . . MAIN.DAT

MODPATH and MODPATH-PLOT (version 3.x)

Main data file MAIN30.DAT
(Other files required by MODPATH, such as RIV.DAT or WEL.DAT are the same as those of MODFLOW.)

MOC3D

Main MOC3D Package . . . . . MOCMAIN.DAT
Source Concentration in Recharge . . . . . MOCCRCH.DAT
Observation Well File . . . . . MOCOBS.DAT

MT3D

Advection Package MTADV1.DAT
Basic Transport Package MTBTN1.DAT
Chemical Reaction Package MTRCT1.DAT
Dispersion Package MTDSP1.DAT
Sink & Source Mixing Package MTSSM1.DAT

MT3DMS

Advection Package MTMSADV1.DAT
Basic Transport Package MTMSBTN1.DAT
Chemical Reaction Package MTMSRCT1.DAT

Dispersion Package MTMSDSP1.DAT
Generalized Conjugate Gradient Solver MSMSGSG1.DAT
Sink & Source Mixing Package MTMSSSM1.DAT

PEST

Instruction File . . . . . INSTRUCT.DAT
Control File . . . . . PESTCTL.DAT
Block-Centered Flow Package Template File . . . . . BCFTPL.DAT
Drain Package Template File . . . . . DRNTPL.DAT
Evapotranspiration Package Template File . . . . . EVTTPL.DAT
General-Head Boundary Package Template File . . . . . GHBTPL.DAT
Recharge Package Template File . . . . . RCHTPL.DAT
River Package Template File . . . . . RIVTPL.DAT
Well Package Template File . . . . . WELTPL.DAT
Stream-Routing Flow Package Template File . . . . . STRTPL.DAT
Interbed-Storage Package Template File . . . . . IBSTPL.DAT
Grid Specification File (used by MODBORE.EXE) . . . . . *filename*.GRD*
Borehole Listing File (used by MODBORE.EXE) . . . . . BORELIST.DAT
Borehole Coordinates File (used by MODBORE.EXE) . . . . . BORECOOR.DAT

* See appendix 2 for the format of the grid specification file

UCODE

Prepare File . . . . . UCODE.PRE
Universal File . . . . . UCODE.UNI
Extract File . . . . . UCODE.EXT
Block-Centered Flow Package Template File . . . . . BCFTPL.DAT
Drain Package Template File . . . . . DRNTPL.DAT
Evapotranspiration Package Template File . . . . . EVTTPL.DAT
General-Head Boundary Package Template File . . . . . GHBTPL.DAT
Recharge Package Template File . . . . . RCHTPL.DAT
River Package Template File . . . . . RIVTPL.DAT
Well Package Template File . . . . . WELTPL.DAT
Stream-Routing Flow Package Template File . . . . . STRTPL.DAT
Interbed-Storage Package Template File . . . . . IBSTPL.DAT
Grid Specification File (used by MODBORE.EXE) . . . . . *filename*.GRD*
Borehole Listing File (used by MODBORE.EXE) . . . . . BORELIST.DAT
Borehole Coordinates File (used by MODBORE.EXE) . . . . . BORECOOR.DAT

Appendix 4: Internal data files of PMWIN

PMWIN saves most of the user-specified data in binary files by using the model name as the file name and the extensions given in the following lists. Cell-by-cell data are saved in files indicated by CBC. Zone data are saved in files indicated by ZONE. The data files with the same file type (e.g., CBC or ZONE) are saved in the same format. The source code (in the Visual Basic 6 format) for the input and output of the CBC files can be found in the folder \source\array_io\ of the companion CD-ROM.

Geometry and Boundary Conditions

Extension	Type	Description
XY	ASCII	Cell sizes and numbers of cells and layers
BOT	CBC	Elevation of the bottom of layers.
IBD	CBC	IBOUND matrix (used by MODFLOW and MOC3D).
TIC	CBC	ICBUND matrix (used by MT3D and MT3DMS)
TOP	CBC	Elevation of the top of layers.
BOZ	ZONE	Elevation of the bottom of layers**.**
IBZ	ZONE	IBOUND matrix.
TOZ	ZONE	Elevation of the top of layers.

Initial Values

Extension	Type	Description
HEA	CBC	Initial hydraulic heads.
TSC	CBC	Initial concentration used by MT3D and MOC3D.
201 230	CBC	Initial concentration of species #1 to #30 used by MT3DMS.
HEZ	ZONE	Initial hydraulic heads.
MT1	ZONE	Initial concentration.
301 330	ZONE	Initial concentration of species #1 to #30 used by MT3DMS.

Aquifer Parameters

Extension	Type	Description
CON	CBC	horizontal hydraulic conductivity.
HTC	CBC	Transmissivity.
LEA	CBC	Vertical hydraulic conductivity.
LKN	CBC	Vertical leakance.
POR	CBC	Effective porosity.
SCC	CBC	Storage coefficient.
STO	CBC	Specific storage.
TAL	CBC	Longitudinal dispersivity.
YLD	CBC	Specific yield.
63	CBC	Parameter numbers associated with horizontal hydraulic conductivity
64	CBC	Parameter numbers associated with vertical hydraulic conductivity.
65	CBC	Parameter numbers associated with specific storage
66	CBC	Parameter numbers associated with transmissvity
67	CBC	Parameter numbers associated with vertical leakance
68	CBC	Parameter numbers associated with storage coefficient
69	CBC	Parameter numbers associated with specific yield
COZ	ZONE	horizontal hydraulic conductivity.
HTZ	ZONE	Transmissivity.
LEZ	ZONE	Vertical hydraulic conductivity.
LKZ	ZONE	Vertical leakance.
POZ	ZONE	Effective porosity.

SCZ	ZONE	Storage coefficient.
STZ	ZONE	Specific storage.
YLZ	ZONE	Specific yield.
163	ZONE	Parameter numbers associated with horizontal hydraulic conductivity
164	ZONE	Parameter numbers associated with vertical hydraulic conductivity.
165	ZONE	Parameter numbers associated with specific storage
166	ZONE	Parameter numbers associated with transmissvity
167	ZONE	Parameter numbers associated with vertical leakance
168	ZONE	Parameter numbers associated with storage coefficient
169	ZONE	Parameter numbers associated with specific yield

BCF2 Package

Extension	Type	Description
DWA	CBC	Wetting threshold.
DWZ	ZONE	Wetting threshold.

Density Package

Extension	Type	Description
C37	CBC	Cell density.
Z37	ZONE	Zone file

Drain Package

Extension	Type	Description
DRC	CBC	Hydraulic conductance of the interface between an aquifer and a drain.
DRE	CBC	Elevation of drain.
291	CBC	Parameter numbers associated with drains
DCZ	ZONE	Zone file

Evapotranspiration Package

Extension	Type	Description
EET	CBC	Maximum evapotranspiration rate [L/T].
EIE	CBC	Layer indicator array. For each horizontal location, it indicates the layer from which evapotranspiration is removed.
ESU	CBC	Elevation of the evapotranspiration surface.
EXD	CBC	Evapotranspiration extinction depth.
292	CBC	Parameter numbers associated with EVP cells.
ETZ	ZONE	Zone file.

General-Head Boundary Package

Extension	Type	Description
GHB	CBC	Head on the general-head-boundary.
GHC	CBC	Hydraulic conductance of the interface between the aquifer cell and the general-head boundary.
293	CBC	Parameter numbers associated with GHB cells.
GCZ	ZONE	Zone file

Horizontal-Flow Barriers Package

Extension	Type	Description
WAL	CBC	Direction of a horizontal-flow barrier.
WAC	CBC	Hydraulic conductivity divided by the thickness of a horizontal-flow barrier.

Interbed Storage Package

Extension	Type	Description
IB1	CBC	Preconsolidation Head.
IB2	CBC	Elastic Storage Factor.
IB3	CBC	Inelastic Storage Factor.
IB4	CBC	Starting Compaction.
294	CBC	Parameter numbers associated with IBS cells.
I1Z	ZONE	Zone file.

Recharge Package

Extension	Type	Description
RCH	CBC	Recharge flux [L/T].
RCI	CBC	Layer indicator array that defines the layer in each vertical column where recharge is applied.
295	CBC	Parameter numbers associated with recharge.
RHZ	ZONE	Zone file.

Reservoir Package

Extension	Type	Description
C85	CBC	Location of reservoirs.
C86	CBC	Bottom elevation of reservoir.
C87	CBC	Bed conductivity of reservoir.
C88	CBC	Bed thickness of reservoir.
C89	CBC	Layer indicator of reservoir.
296	CBC	Parameter numbers associated with reservoir cells.
Z85	Zone	Zone file.

River Package

Extension	Type	Description
RIC	CBC	Hydraulic conductance of riverbed.
RIR	CBC	Elevation of the bottom of riverbed.
RIS	CBC	Water surface elevation of river.
297	CBC	Parameter numbers associated with River cells.
RCZ	ZONE	Zone file

Streamflow-Routine Package

Extension	Type	Description
SBO	CBC	Elevation of the bottom of the streambed.
SEG	CBC	Segment number - sequential number assigned to a group of reaches.
SFL	CBC	Streamflow in length cubed per time.
SRE	CBC	Sequential number of reaches.
SRO	CBC	Manning's roughness coefficient/C for each stream reach.

SSL	CBC	Slope of the stream channel in each reach.
SST	CBC	Stream stage.
STC	CBC	Streambed hydraulic conductance.
STT	CBC	Elevation of the top of the streambed.
SWI	CBC	Width of the stream channel in each reach.
298	CBC	Parameter numbers associated with stream cells.
S1Z	ZONE	Zone file.

Time Variant Specified Head (CHD) Package

Extension	Type	Description
CH1	CBC	A non-zero value indicates a CHD cell.
CH2	CBC	Head at the beginning of a stress period (Start head).
CH3	CBC	Head at the end of a stress period (End head).
C1Z	ZONE	Zone file.

Well Package

Extension	Type	Description
WEL	CBC	Volumetric recharge rate of wells.
299	CBC	Parameter numbers associated with Well cells.
WEZ	ZONE	Volumetric recharge rate of wells.

MT3D - Advection Package

Extension	Type	Description
ADV	ASCII	User-specified settings for the Advection Package.

MT3D - Dispersion Package

Extension	Type	Description
DPS	ASCII	User-specified settings for the Dispersion Package.
TAL	CBC	Longitudinal dispersivity.
M11	ZONE	Longitudinal dispersivity.

MT3D - Chemical Reaction Package

Extension	Type	Description
CHE	ASCII	User-specified settings for the Chemical Reaction Package.
C91	CBC	Bulk density (only used by MT3D96).
C92	CBC	First sorption constant (only used by MT3D96).
C93	CBC	Second sorption constant (only used by MT3D96).
C94	CBC	First-order rate constant for the dissolved phase (only used by MT3D96).
C95	CBC	First-order rate constant for the sorbed phase (only used by MT3D96).
Z91	Zone	Zone file containing the chemical reaction parameters for MT3D96.

MT3D - Sink & Source Mixing Package

Extension	Type	Description
TCH	CBC	Specified concentration at constant head cells.
TE	CBC	Specified concentration of evapotranspiration flux.

TG	CBC	Specified concentration at general-head boundary cells.
TR	CBC	Specified concentration of river.
TRC	CBC	Specified concentration of recharge flux.
TST	CBC	Specified concentration of stream.
TW	CBC	Specified concentration of injection wells.
C54	CBC	Flag indicates a Time-variant specified concentration.
C55	CBC	Concentration in a Time-variant specified concentration cell.
MT3	ZONE	Specified concentration of injection wells.
MT5	ZONE	Specified concentration of river.
MT6	ZONE	Specified concentration of evapotranspiration flux.
MT7	ZONE	Specified concentration at general-head boundary cells.
MT8	ZONE	Specified concentration of recharge flux.
MT9	ZONE	Specified concentration of stream.
M10	ZONE	Specified concentration at constant head cells.
Z54	ZONE	Time-variant specified concentration.

MOC3D

Extension	Type	Description
MOC	ASCII	Subgrid, initial concentration outside of the subgrid and dispersion and retardation factor.
MPP	ASCII	Relative position of initial particles.
C57	CBC	Observation wells.
C58	CBC	Strong/Weak flag.
Z57	ZONE	Observation wells.
Z58	ZONE	Strong/Weak flag.
TW	CBC	Specified concentration of injection wells (shared with MT3D).
TG	CBC	Specified concentration at general-head boundary cells (shared with MT3D).
TR	CBC	Specified concentration of river (shared with MT3D).
TRC	CBC	Specified concentration of recharge flux (shared with MT3D).
MT3	ZONE	Specified concentration of injection wells (shared with MT3D).
MT7	ZONE	Specified concentration at general-head boundary cells (shared with MT3D).
MT5	ZONE	Specified concentration of river (shared with MT3D).
MT8	ZONE	Specified concentration of recharge flux (shared with MT3D).

MT3DMS

Extension	Type	Description
231...260	CBC	Concentraion of species #1 to #30 associated with the recharge.
261...290	CBC	Concentraion of species #1 to #30 associated with the evapotranspiration.
401...430	CBC	First sorption constant of species #1 to #30.
431...460	CBC	Second sorption constant of species #1 to #30.
461...490	CBC	First-order rate constant for the dissolved phase of species #1 to #30.
601...630	CBC	First-order rate constant for the sorbed phase of species #1 to #30.
631...660	CBC	Specified concentration of species #1 to #30 at constant head cells.
661...690	CBC	Specified concentration of species #1 to #30 at general-head boundary cells.
801...830	CBC	Specified concentration of species #1 to #30 associated with injection wells.
831...860	CBC	Specified concentration of species #1 to #30 associated with river cells.
861...890	CBC	Specified concentration of species #1 to #30 associated with stream cells.
1001..1030	CBC	Flag indicates a Time-variant specified concentration for species #1 to #30.
1031..1060	CBC	Concentration of species #1 to #30 in a Time-variant specified concentration cell.
1201...1230	CBC	Initial concentraion for the sorbed phase of species #1 to #30.
331...360	ZONE	Concentraion of species #1 to #30 associated with the recharge.
361...390	ZONE	Concentraion of species #1 to #30 associated with the evapotranspiration.
501...530	ZONE	First sorption constant of species #1 to #30.
531...560	ZONE	Second sorption constant of species #1 to #30.

561...590	ZONE	First-order rate constant for the dissolved phase of species #1 to #30.
701...730	ZONE	First-order rate constant for the sorbed phase of species #1 to #30.
731...760	ZONE	Specified concentration of species #1 to #30 at constant head cells.
761...790	ZONE	Specified concentration of species #1 to #30 at general-head boundary cells.
901...930	ZONE	Specified concentration of species #1 to #30 associated with injection wells.
931...960	ZONE	Specified concentration of species #1 to #30 associated with river cells.
961...990	ZONE	Specified concentration of species #1 to #30 associated with stream cells.
1101..1130	ZONE	Flag indicates a Time-variant specified concentration for species #1 to #30.
1131..1160	ZONE	Concentration of species #1 to #30 in a Time-variant specified concentration cell.
1301...1330	ZONE	Initial concentration for the sorbed phase of species #1 to #30.

Other Reserved File Extensions

Extension	Type	Description
PM5	ASCII	Most options and settings of a model are saved in this file.
L	ASCII	Settings of the Layer options.
GRD	ASCII	Grid Specification file (see Appendix 2 for the format)
C97	CBC	Digitizer
Z97	ZONE	Digitizer
_83	CBC	Presentation
Z83	ZONE	Presentation
WBL	CBC	subregions for the calculation of water budget
WEZ	ZONE	subregions for the calculation of water budget
POL	BINARY	contains boreholes and observations (saved automatically by PMWIN).
PPL	BINARY	parameter list for PEST (saved automatically by PMWIN).
UPL	BINARY	parameter list for UCODE (saved automatically by PMWIN).
TRN	BINARY	is a time parameter file (saved automatically by PMWIN).
TRS	BINARY	is a Trace file saved automatically by PMWIN.
TMP		RESERVED for internal use
{T}		RESERVED for internal use

Appendix 5: Using PMWIN with your MODFLOW

PMWIN supports various versions of MODFLOW by using different IUNIT assignments as shown in Table 7.1. These IUNIT assignments must be the same as those used in the main program of your own version of MODFLOW (see Table 7.2 for an example). In the Run Modflow dialog box, you may select any MODFLOW version to use with your own MODFLOW program, as long as the IUNIT assignments match the default values shown in Table 7.1.

Table 7.1 Default settings of the IUNIT assignments

MODFLOW Version / Package	MODFLOW (MODFLOW-88)	MODFLOW-96	PMWIN 4.X [1]	User' Own
BCF (BCF2)	1	1	1	1
Well	2	2	2	2
Drain	3	3	3	3
River	4	4	4	4
Evapotranspiration	5	5	5	5
General-head boundary	7	7	7	7
Recharge	8	8	8	8
SIP	9	9	9	9
DE45 [2]	10	10	10	10
SSOR	11	11	11	11
Output Control	12	12	12	12
PCG2	13	13	13	13
Horizontal-Flow Barriers	14	16	14	14
Reservoir	16	17	16	16
Streamflow Routing	17	18	17	17
Interbed Storage	19	19	19	19
Time Variant Specified Head	20	20	20	20
Density [3]	21	-	-	-
LKMT	22	22	22	22

1: This version of MODFLOW uses dynamic memory allocation and allows pratically unlimited number of cells.
2: DE45 is not supported by the KIWA-version of MODFLOW.
3: The Density Package is a proprietary software and is contained only in the KIWA-version of MODFLOW. Use of this software is royalty free. The source code is, however, not contained in PMWIN.

Table 7.2 IUNIT assignments given in the main program of MODFLOW

```
      IF(IUNIT(1).GT.0) CALL BCF2AL(ISUM,LENX,LCSC1,LCHY,
     1    LCBOT,LCTOP,LCSC2,LCTRPY,IUNIT(1),ISS,
     2    NCOL,NROW,NLAY,IOUT,IBCFCB,LCWETD,IWDFLG,LCCVWD,
     3    WETFCT,IWETIT,IHDWET,HDRY)
      IF(IUNIT(2).GT.0) CALL WEL1AL(ISUM,LENX,LCWELL,MXWELL,NWELLS,
     1            IUNIT(2),IOUT,IWELCB)
      IF(IUNIT(3).GT.0) CALL DRN1AL(ISUM,LENX,LCDRAI,NDRAIN,MXDRN,
     1            IUNIT(3),IOUT,IDRNCB)
      IF(IUNIT(4).GT.0) CALL RIV1AL(ISUM,LENX,LCRIVR,MXRIVR,NRIVER,
     1          IUNIT(4),IOUT,IRIVCB)
      IF(IUNIT(5).GT.0) CALL EVT1AL(ISUM,LENX,LCIEVT,LCEVTR,LCEXDP,
     1          LCSURF,NCOL,NROW,NEVTOP,IUNIT(5),IOUT,IEVTCB)
      IF(IUNIT(7).GT.0) CALL GHB1AL(ISUM,LENX,LCBNDS,NBOUND,MXBND,
     1          IUNIT(7),IOUT,IGHBCB)
      IF(IUNIT(8).GT.0) CALL RCH1AL(ISUM,LENX,LCIRCH,LCRECH,NRCHOP,
     1          NCOL,NROW,IUNIT(8),IOUT,IRCHCB)
      IF(IUNIT(9).GT.0) CALL SIP1AL(ISUM,LENX,LCEL,LCFL,LCGL,LCV,
     1         LCHDCG,LCLRCH,LCW,MXITER,NPARM,NCOL,NROW,NLAY,
     2         IUNIT(9),IOUT)
      IF(IUNIT(11).GT.0) CALL SOR1AL(ISUM,LENX,LCA,LCRES,LCHDCG,LCLRCH,
     1          LCIEQP,MXITER,NCOL,NLAY,NSLICE,MBW,IUNIT(11),IOUT)
      IF(IUNIT(13).GT.0) CALL PCG2AL(ISUM,LENX,LCV,LCSS,LCP,LCCD,
     1       LCHCHG,LCLHCH,LCRCHG,LCLRCH,MXITER,ITER1,NCOL,NROW,NLAY,
     2       IUNIT(13),IOUT,NPCOND)
      IF(IUNIT(14).GT.0) CALL STR1AL(ISUM,LENX,LCSTRM,ICSTRM,MXSTRM,
     1            NSTREM,IUNIT(14),IOUT,ISTCB1,ISTCB2,NSS,NTRIB,
     2              NDIV,ICALC,CONST,LCTBAR,LCTRIB,LCIVAR)
      IF(IUNIT(16).GT.0) CALL HFB1AL(ISUM,LENX,LCHFBR,NHFB,IUNIT(16),
     1          IOUT)
      IF(IUNIT(19).GT.0) CALL IBS1AL(ISUM,LENX,LCHC,LCSCE,LCSCV,
     1          LCSUB,NCOL,NROW,NLAY,IIBSCB,IIBSOC,ISS,IUNIT(19),IOUT)
      IF(IUNIT(20).GT.0) CALL CHD1AL(ISUM,LENX,LCCHDS,NCHDS,MXCHD,
     1          IUNIT(20),IOUT)
```

Appendix 6: Running MODPATH with PMWIN

PMWIN supports both two versions (version 1.x and 3.x) of MODPATH and MODPATH-PLOT. You must run MODPATH or MODPATH-PLOT within a DOS-Box (of Windows) or in the DOS-Environment.

If you are using MODPATH version 1.x (released prior to September, 1994), type ***path*\PATHFILE** at the prompt **ENTER NAME OF FILE CONTAINING NAMES AND UNITS OF DATA FILES.** Where *path* is the path to the directory of your model data. PATHFILE contains the IUNIT assignments and paths and names of input data files generated by PMWIN. The names of the input files for MODFLOW and MODPATH are given in Appendix 7.

If you are using MODPATH or MODPATH-PLOT (version 3.x), follow the steps below:

TO READ INPUT FROM AN EXISTING RESPONSE FILE, ENTER FILE NAME:
(<CR> = ENTER DATA INTERACTIVELY)
[? = Help]

(WHAT YOU SHOULD DO: Just press ENTER here. For the first time you run MODPATH or MODPATH-PLOT, you do not have a response file and you have to enter data interactively. The user-specified data will be saved by MODPATH or MODPATH-PLOT in the response files MPATH.RSP or MPLOT.RSP, respectively. Using a response file, you do not need to go through the input procedures unless you want to change the data for MODPATH or MODPATH-PLOT).

Only for MODPATH-PLOT:
TO REDEFINE SETTINGS, ENTER NAME OF FILE WITH SETTINGS DATA:
(<CR> = USE DEFAULT SETTINGS FOR DEVICE)
[? = Help]

(WHAT YOU SHOULD DO: Just press ENTER here, unless you want to change settings.)

ENTER THE NAME FILE:
[? = Help]

(WHAT YOU SHOULD DO: Type *path*\MPATH30 at this prompt. Where *path* is the path to the directory of your model data. For example, if you have saved your model data in C:\PMWIN\DATA, you will type C:\PMWIN\DATA\MPATH30 at this prompt. After this prompt, you enter the interactive input procedure of MODPATH or MODPATH-PLOT. Just follow the prompts of the programs.)

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