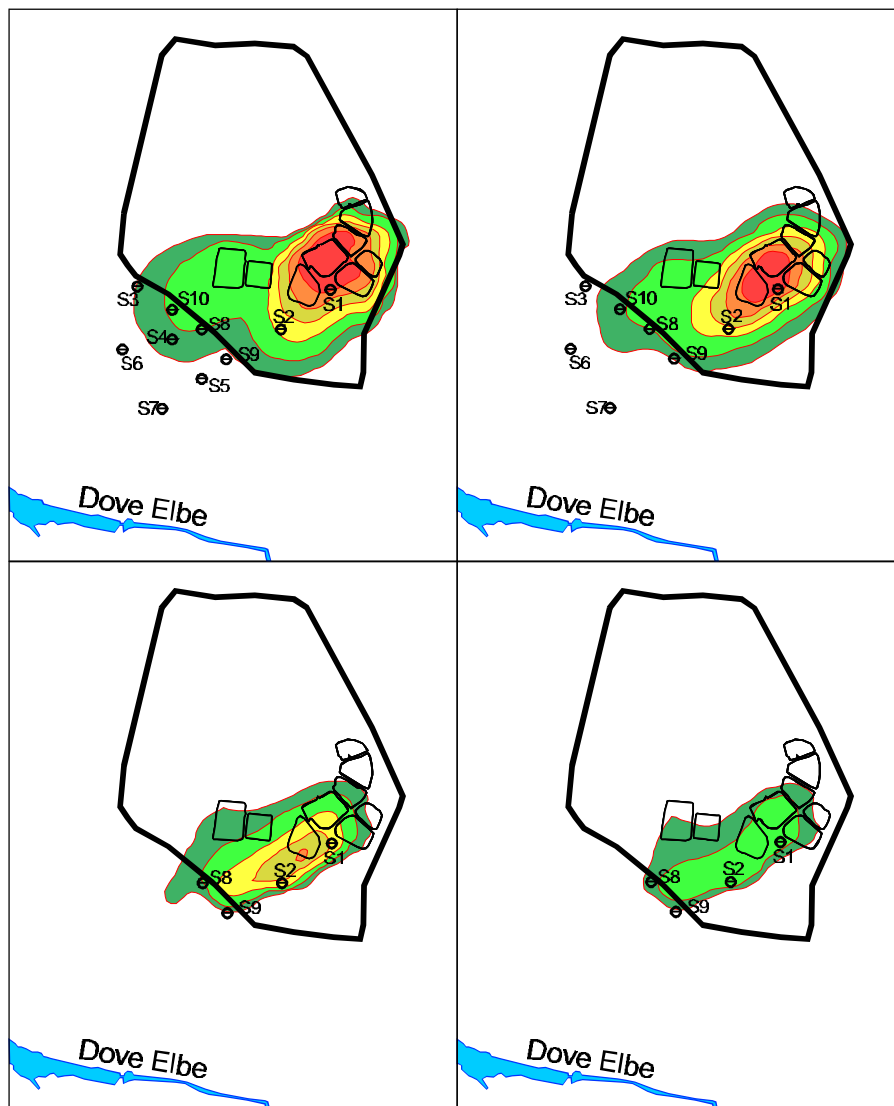# PROCESSING MODFLOW

Pre- and Postprocessors for Simulation of
Flow and Contaminants Transport in Groundwater Systems with
MODFLOW, MODPATH and MT3D

Version 3.0

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Table of Contents

5. Simulation of Groundwater Flow and Solute Transport

6. Postprocessors

Appendices

A. Application

B. Input data files for the simulation models

C. Data files used internally by **PM**

D. Limitations of the preprocessors

E. Using the grid editor to import/export data

F. Continuation of a previous run

References

Preface

This document describes the use of **PROCESSING MODFLOW (PM)** in conjunction with the U.S. Geological Survey's modular groundwater flow model MODFLOW (McDonald and Harbaugh, 1988; Prudic, 1989), the particle tracking program MODPATH (Pollock, 1988) and the transport model MT3D (Zheng, 1990). It is assumed that users have an adequate theoretical background on the groundwater flow and transport processes. Detailed explanations of physical and mathematical concepts on which the models are based and explanations of how those concepts were incorporated in the computer programs will not be discussed in this document. They can be found in the corresponding documentations of the computer programs.

Due to its intensive graphical facilities, **PM** is suitable for both professional and educational purposes. We hope that the pre- and postprocessors provided by this software will help modelers or students in constructing groundwater models, understanding the behavior of the considered systems and solving the flow and pollution problems.

Many thanks are due to Prof. René Therrien (Dept. of Earth and Planetary Sciences, McGill University, Montréal) for his helpful discussions and contributions in developing this software.

<div align="right">

Wen-hsing Chiang
Wolfgang Kinzelbach

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1. Introduction

1.1 Objective and scope

In recent years, numerous analytical and numerical groundwater models have been used to simulate the behavior of groundwater systems. Analytical models, such as PAT (Kinzelbach and Rausch, 1991), can be used to simulate groundwater flow and transport for aquifers with simple initial and boundary conditions. However, for most cases of practical interest, the analytical method cannot be used feasible because of the heterogeneity of the aquifer parameters (e.g., hydraulic conductivity), irregular shape of the domain boundaries and irregular temporal and spatial distributions of the various sink-sources functions. Numerical models, which are in majority based on methods of finite elements or finite differences, have been therefore developed and are widely used to simulate aquifer systems with more complex initial and boundary conditions. Although numerical models are flexible and powerful, the construction of such a model is time-consuming because of the large amount of input data required. This is especially true in three dimensions. Hence, many numerical models, for example ASM (Kinzelbach et al., 1989), GFR (Chiang, 1993) or AQUA (Vatnaskil Consulting Engineers, 1989) provide their own graphical preprocessor and postprocessors.

However, user-friendly graphical preprocessors and postprocessors are not provided by the U.S. Geological Survey's modular groundwater flow model MODFLOW (McDonald and Harbaugh, 1988), the particle tracking model MODPATH (Pollock, 1988) and the transport model MT3D (Zheng, 1990). Without a graphical user interface (GUI), the use of such models is sometimes very cumbersome. **PROCESSING MODFLOW (PM)** is developed in this way to help the modeler perform numerical groundwater simulations with these models. More programs, which run with MODFLOW, have recently been developed by a large number of researchers. For example, MODFLOW/P (Hill, 1992) for solving the inverse problems, MODWALK (Schäfer, 1993) for simulating contaminant transport by using the Random Walk method. These programs will be supported in a future version of **PM**.

1.2 Organization of PM and this manual

PM consists of three parts: preprocessors, simulation models[1] and postprocesssors. Fig. 1.1

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[1] the simulation models MODFLOW, MODPATH/MODPATH-PLOT and MT3D are supported but not included in **PM**.

shows the organizational chart of **PM**. All programs and models shown in Fig. 1.1 can be called from **PM** by selecting a corresponding menu item from the pull-down menus of the PM-shell (Fig. 1.2). For example, one can run the preprocessor for MODFLOW by selecting the menu item "edit flow model" or the preprocessor for MT3D by selecting the menu item "edit transport model". All preprocessors and postprocessors provided by **PM** also have a menu-driven user interface and feature extensive graphics and data processing capabilities, e.g., import and export of DXF-maps and data matrices. Through the easy-to-understand menu system and the graphical user interface (GUI), the use of **PM** is extremely easy.
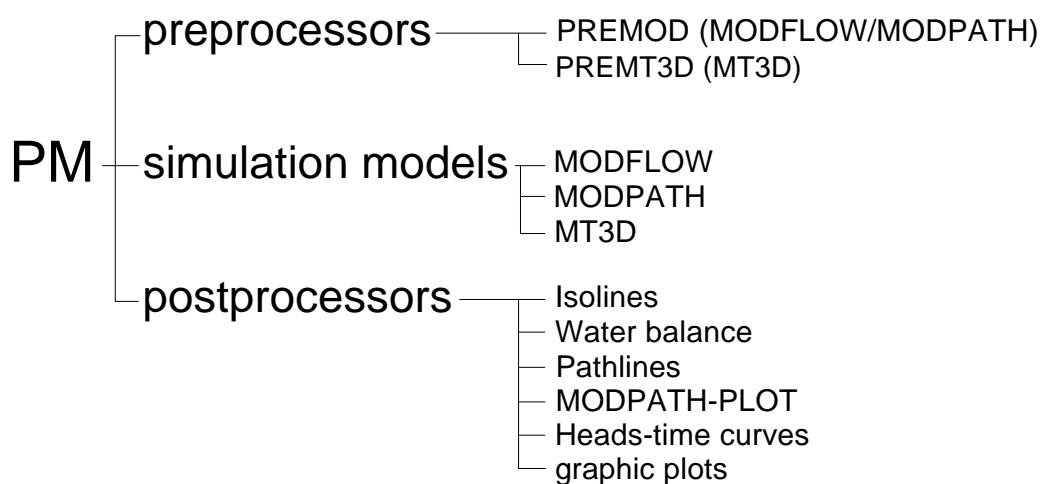

Fig. 1.1: The organizational chart of **PM**
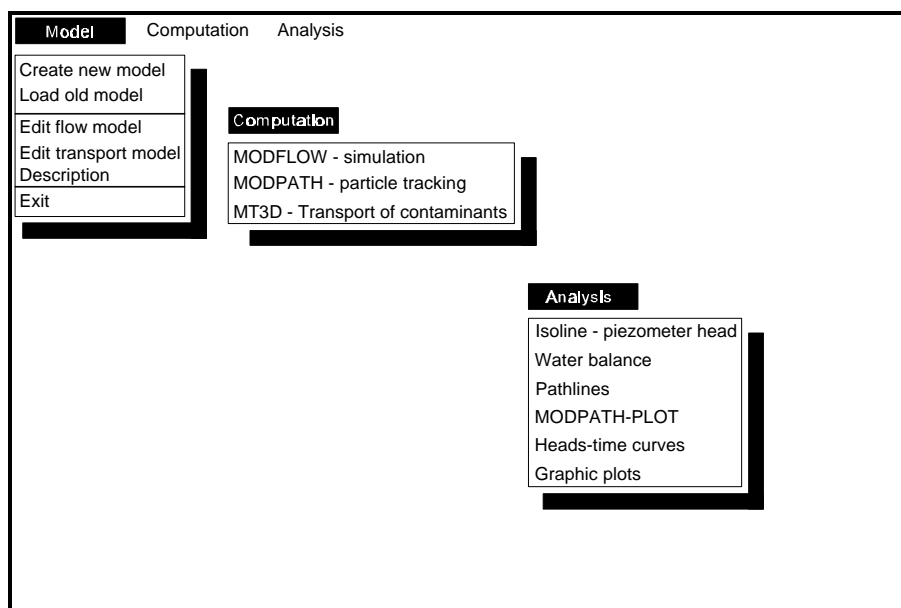
Fig. 1.2: The pull-down menus of the **PM**-shell

Following is a simplified chart, which explains how **PM** works:

Preprocessors

By using the preprocessors, model data will be specified. To save time and hard disk space, **PM** internally saves model data in binary files. Through translators, the binary model data files are converted into ASCII files, which can be accepted by the simulation models.

Simulation models

Simulation models, which are supported by **PM**, can be called from the PM-shell. One can perform groundwater simulations without leaving **PM**. In most cases, simulation results of MODFLOW will be saved in four files - a simulation report file and three unformatted heads, drawdown and budget files. Some of these files will be used by MOD-PATH for calculating pathlines in a steady state three-dimensional flow field. The result files of MODFLOW and MODPATH will be used by the postprocessors. MT3D generates a standard report file and several optional output files. Some of the optional output files will be used by the postprocessor provided by MT3D and **PM**.

Postprocessors

The postprocessors permit the calculation of the sub-regional water balance and create graphical plots of simulation results, e.g., pathlines, isolines of the piezometer heads or concentration distribution or heads-time curves. The areally distributed input data, such as hydraulic conductivity or porosity, can also be displayed in form of contours or classes for each model layer. The graphics can be used for representations or for controlling purpose.

This manual describes the use of **PM** in conjunction with the models and programs supported or provided by **PM**. The use of each menu item of all pull-down menus will be described in detail. The index of menu items attached at the end of this manual indicates to the user where she/he can find the description of a menu item.

Detailed explanations of physical and mathematical concepts on which the models are based and explanations of how those concepts were incorporated in the computer programs will not be discussed in this document. They can be found in the corresponding documentations of the

computer programs. Theories and applications for modeling of groundwater in porous media can also be found in numerous publications (e.g., Bear et al., 1987; Kinzelbach, 1986, 1992).

The following chapters provide detailed information about the use of **PM.**

- Chapter 2 explains how to install **PM**.

- Chapter 3 describes the use of the PM-shell.

- Chapter 4 describes the preprocessors for MODFLOW and MT3D. In this chapter, you will learn how to use the build-in CAD features to construct a map of the model area, and how to use the grid editor and zones-editor provided by **PM** for specifying the model data.

- Chapter 5 discusses the simulation models and provides detailed explanations for running these models within **PM**.

- Chapter 6 describes the use of postprocessors. In this chapter, you will learn how to use the postprocessors to create graphic plots and to calculate water balances. This chapter also explains each option, discusses how an option can be selected and notes its potential uses.

- The appendices contain a description of the example model of **PM**, basic information pertaining to the IUNIT location assignments, data files used or created for the simulation models and the size limitation of a model created by **PM**.

2. Getting Started

This chapter describes how to install **PM** on a 386/387 or 486DX-based computer. Before starting, it is suggested to make working copies of your **PM**-diskettes.

2.1 System requirements

You must have:

- **Hardware:**
  - ✓ An 80386/387- or 80486DX-based IBM Personal Computer or compatible with an EGA- or VGA-graphics card and at least 550 KB of free conventional and 2 MB of extended memory.
  - ✓ Microsoft Mouse or compatible
  - ✓ A hard disk with at least 5 MB of free space for **PM** (and since model data take considerable space, a 20 MB minimum work space is recommended).
  - ✓ optional:
    If only preprocessing facilities are used, an 80286-based IBM Personal Computer or compatible is sufficient.

- **Software:**
  - ✓ Operating system MS-DOS 3.1 or later.
  - ✓ Microsoft Mouse driver. Although many manufacturers advertise their mouse as being compatible with the Microsoft Mouse, **PM** will work properly only when a 100% compatible mouse driver is installed. The original Microsoft Mouse driver is therefore recommended. There are two drivers available: MOUSE.COM and MOUSE.SYS. They can be found in almost all Microsoft products (e.g., WINDOWS 3.1).
  - ✓ Optional:
    Lahey Fortran compiler (F77L EM/32), only if changes in the Fortran source code are intended.

2.2 Installing PM

This section walks you through the installation of **PM**. Don't worry if you are not experienced at installing software, **PM** will prompt you for any information you will need. To install **PM**:

1. Insert the PM distribution diskette labelled "Installation & Modeling 1" in the floppy drive A (or B), change the default drive to this drive, type INSTALL at the DOS-prompt then press ENTER.

2. The **PM** installation program dialog box will come up, and ask for the drive and path where you want **PM** installed. If you wish to use the default directory C:\PM, click "OK". Otherwise, use the backspace to erase the default directory, and type in the full path name of your choice, and then click "OK".

3. Another dialog box will come up and ask for a version of the BCF Package and a version of distributed MODFLOW. You can choose the options by using the mouse or the TAB-key and the SPACE BAR. Click "OK", after having chosen the options. Currently, **PM** can be installed to run with the version of MODFLOW distributed by the Scientific Software Group (SSG), the International Ground Water Modeling Center (IGWMC) and the S. S. Papadopulos & Associates, Inc. (SSPA), without having to make any change in the simulation models. **PM** will also run with your own MODFLOW, as long as the program has the same input routines as the "original" MODFLOW (McDonald et al, 1988). After having installed **PM**, the filenames listed in Tab. 2.1 will be used by the PM-shell for calling the simulation models.

4. **PM** will install the necessary files from the floppy diskettes and prompt you to insert the other diskettes, if they are needed.

5. When finished, a dialog box will appear with information about the simulation programs, which can be called from the PM-shell. Click "OK", to return to DOS.

With **PM** installed, you are ready to begin constructing three dimensional groundwater flow and transport models. **Please note that MODFLOW, MODPATH, MODPATH-PLOT and MT3D can be called from the PM-shell, only if they are installed in the same directory as PM.** About the installation of MODFLOW, MODPATH, MODPATH-PLOT and MT3D, please refer to the corresponding installation guide from the software manufacturers.

Software-version	SSG	IGWMC	SSPA	User's
MODFLOW	MFLOWEM.EXE	MOD-EM.EXE	MODF.EXE	MODFLOW.EXE
MODPATH	MPATHEM.EXE	MPATHEM.EXE	MPATHEM.EXE	MPATHEM.EXE
MODPATH-PLOT	MPLOTEM.BAT	MPLOTEM.BAT	MPLOTEM.BAT	MPLOTEM.BAT
MT3D	MT3D.EXE	MT3D.EXE	MT3D.EXE	MT3D.EXE

Tab. 2.1: Filenames used by the PM-shell for calling the simulation models

2.3 Starting PM

To start **PM**, change to the PM directory and type "PM3" at the DOS prompt and then press <ENTER>. The introduction screen appears (Fig. 2.1). To proceed to PM-shell, press any key.

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Version 3.0

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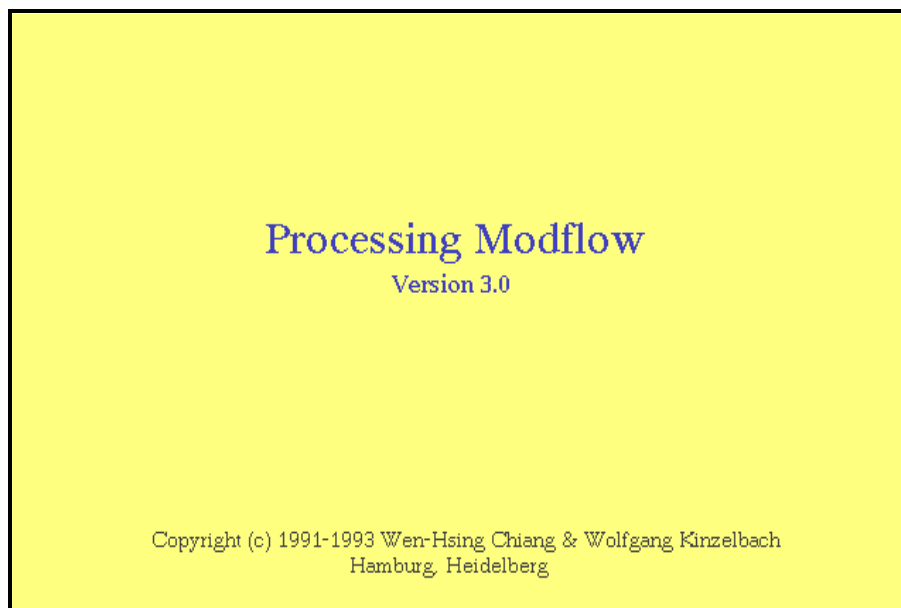
Fig. 2.1: The introduction screen of **PM**

3. The PM-shell

3.1 The PM-shell menus

PM uses "pull-down" menus as shown in Fig. 3.1. The menu bar of the PM-shell at the top of the screen contains three menu titles. The status line at the bottom of the screen shows the model currently being used. This line vanishes if no model is loaded or created. To pull down a menu, press the ALT-key and use the arrow keys to highlight a menu title, then press the ENTER-key. For your convenience, you can also pull down a menu by clicking the mouse on a menu title and then click the mouse on a menu item to select it.
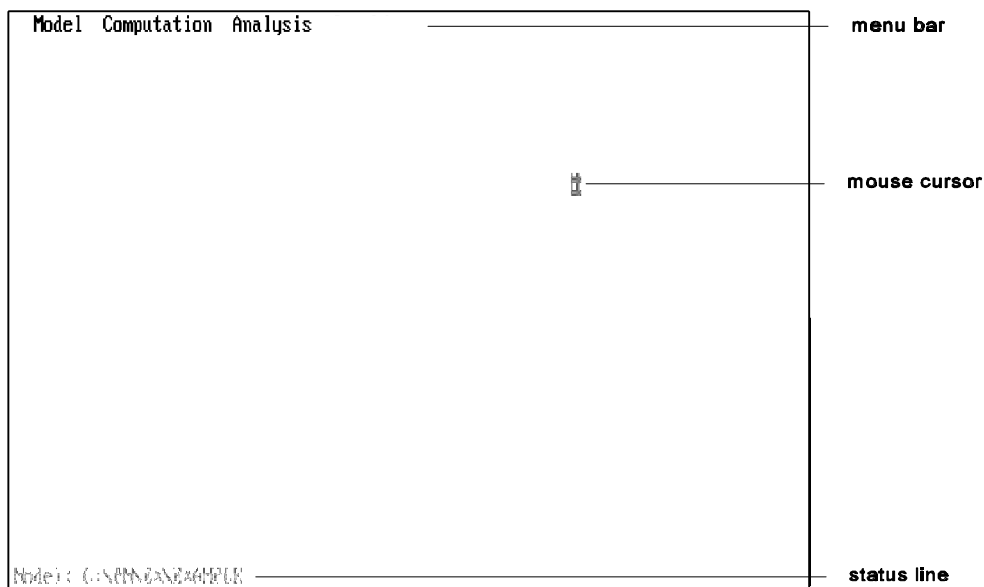
Fig. 3.1: The PM-shell menus

3.2 The "Model" menu

Fig. 3.2 shows the "Model" menu. The menu items are described below:

Create new model
The first step of applying **PM** is to create a new model. This is done by selecting this menu item. A dialog box will come up and ask for the path and file name. All filenames valid under MS-DOS can be used. The filename without path may consist of at most 8 characters and must be entered without extension.
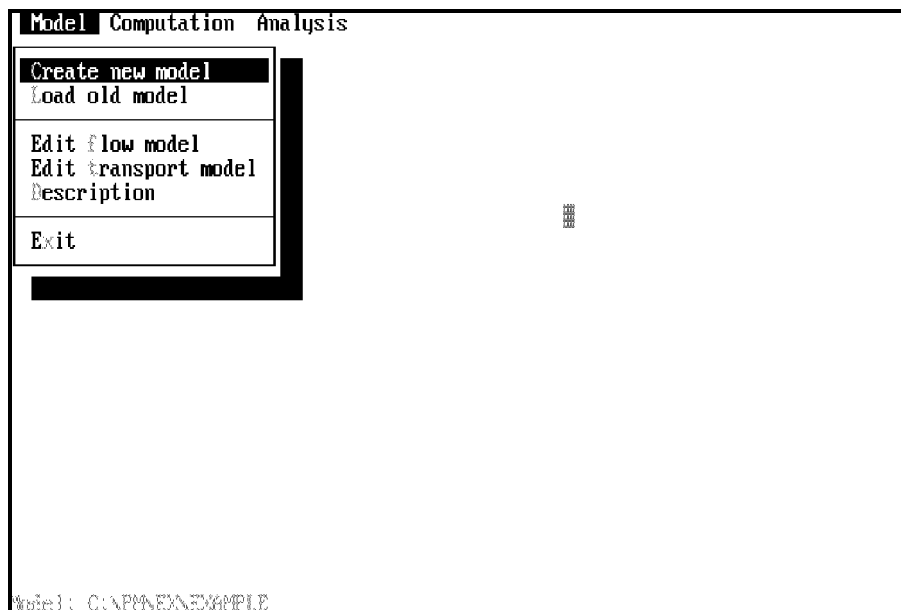
Fig. 3.2: The "Model" menu

Load old model

Once you have created a model (and specified model data), you can subsequently reload and modify this model. Similar to the "Create new model" option, a dialog box will ask for the path and file name of the model to be loaded. After having created or loaded a model, the model filename and the full path will be displayed on the status line.

Edit flow model

To prepare data for the flow model, i.e. data for MODFLOW, select this menu item. The preprocessor for MODFLOW - PREMOD will be loaded.

Edit transport model

To prepare data for the transport model, i.e. data for MT3D, select this menu item. The preprocessor for MT3D - PREMT3D will be loaded. Please note that the data for the flow model should be complete before preparing data for the transport model. This is not a limitation of **PM**; it is due to the fact that MT3D is designed to be used in conjunction with a block-centered finite-difference flow model, such as MODFLOW. Prior to running MT3D, the heads, fluxes across cell interfaces in all directions and locations and flow rates for the various sinks/sources must be solved by the flow model.

Description

To write a description of a model, select this menu item. The description will be printed in the simulation report file.

Exit

As you might expect, this menu item allows you to exit **PM**.

3.3 The "Computation" menu

The simulation models MODFLOW, MODPATH and MT3D can be called by selecting a corresponding menu item from the "Computation" menu (Fig. 3.3). During the simulation, the PM-shell will be suspended until the simulation run is finished or terminated.

For many reasons, a MODFLOW or MT3D simulation run will sometimes be terminated without any message displayed on the screen. For example, if a criterion for convergence cannot be reached within a time step, MODFLOW will stop the simulation and put a message "Failed to converge in time step ..." in the standard simulation report file, but not on the screen. It is therefore recommended to read the simulation report file or at least glance at it. Furthermore, the report file contains other essential information. In case of difficulty, this supplementary information can be very helpful.

During a MODFLOW or MT3D simulation, heads, drawdowns and concentration fields are saved in unformatted binary files. After the simulation run, the program **PMCNV** or **MT3DCNV** provided by PM will be called to convert the binary files into ASCII. The ASCII files are used by the postprocessors for creating graphic plots of isolines and heads-time curves.
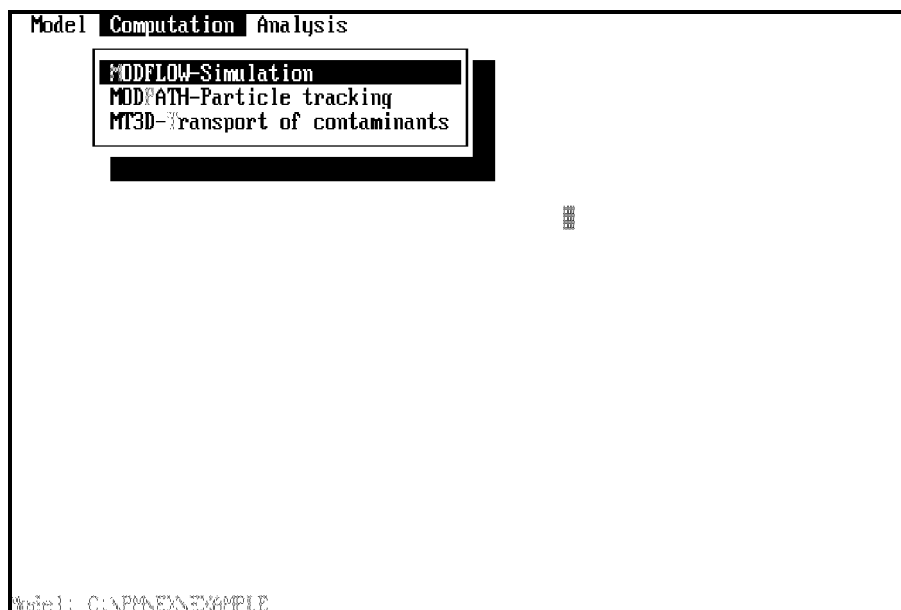
Fig. 3.3: The "Computation" menu

3.4 The "Analysis" menu

PM provides five postprocessors and supports the postprocessor MODPATH-PLOT. The postprocessors can be called by selecting a corresponding menu item from the "Analysis" menu (Fig. 3.4).

Fig. 3.4: The "Analysis" Menu

The following is a short description of each postprocessor; the use of the postprocessors will be described in chapter 6.

Isoline - piezometer heads

The postprocessor **ISOLINE** is designed for the graphic presentation of head and drawdown contours in layers. The region for the presentation of contours, the lower and upper boundaries of the contours and the increment of contours may either be set as default values by **PM** or specified by the user. Optionally, the contours may be saved in HPGL- or DXF-format and as SURFER input file.

Water balance

This postprocessor is developed for the computation of the water balance for arbitrary subregions and for the whole model domain. It uses the unformatted binary cell-by-cell budget output file from MODFLOW. The subregions are defined by the user through the use of the GUI (Graphical User Interface) of **PM**. The table of water balance contains various in- and out-flows for each model layer and for each subregional zone.

MODPATH-PLOT

MODPATH-PLOT (Pollock, 1989) graphically displays the output from MODPATH. It permits display of starting points, ending points, and pathlines in plan view and cross section. This program is not included in **PM**.

Pathlines

The postprocessor **PATHLINE** uses the results of MODPATH to show a 3D-view of pathlines or to draw projections of pathlines on the coordinate planes of the model domain. The graphic plots can be saved in HPGL or DXF files.

Heads-time curves

The postprocessor **PMHT** draws the temporal development curves of the piezometer heads versus time at observation cells. The locations of the observation cells are specified by the user with the help of the GUI. The heads-time curves can be displayed on the screen or optionally saved in HPGL files.

Graphic plots

With the program **PMGRAF**, areally distributed input data, e.g., hydraulic conductivity, porosity or specific storage, can be displayed in form of contours or classes for each layer. The graphics can be saved alternatively in HPGL, DXF format or as SURFER input file. These graphic plots can help you to visually control the input data.

4. Preprocessors

PM provides two preprocessors for specifying input data for each package of MODFLOW/-MODPATH and MT3D. Both preprocessors allow the use of irregularly spaced grids with up to 15,000 cells in a layer, and the entry of data for up to 80 layers and 1000 stress periods. The extensive graphics and data processing capabilities of the preprocessors make the entry of such a large model possible.

The preprocessors and the simulation models use consistent units for input variables. For example, suppose that SECOND is used as unit for time, feet (FT) for length and pound (LB) for mass. Then all data should be expressed in terms of seconds, FT and LB. For that case, the cell length and hydraulic heads would be expressed in FT, hydraulic conductivity in FT/s, pumping rates in FT^3/s, dispersivity in FT, solute concentration in LB/FT^3, and so on.

This chapter deals with the basic use of the preprocessors for preparing model data. One should be aware that a preprocessor is only a tool which helps the user specify the model data through graphics, menus and dialog boxes. In many cases, the knowledge of groundwater hydraulics and theories of contaminant transport in porous media will be required.

4.1 The model designer

The model designer of the preprocessors is developed to help the user graphically specify the model data. The graphical user interface (GUI) of the model designer consists of three programs - PMCAD for constructing a general map of the model area, a grid editor for specifying the data of each model cell individually and a zones editor for specifying the areally distributed physical data in form of zones. These programs will automatically be called from the preprocessors of **PM** whenever they are needed.

4.1.1 PMCAD

PMCAD allows the user to construct a general map of the model area on the model worksheet with the help of the functions shown on the right-hand side of the screen (Fig. 4.1).
The coordinate system used by PMCAD is also shown in this figure. Through the use of the functions, the model grid can be shifted and rotated. PMCAD can display a user-drawn map and up to three DXF-background maps simultaneously. The scale factor and the displacement of a DXF-map can be specified. With these features, the model grid can be overlaid exactly on the

digitized map.
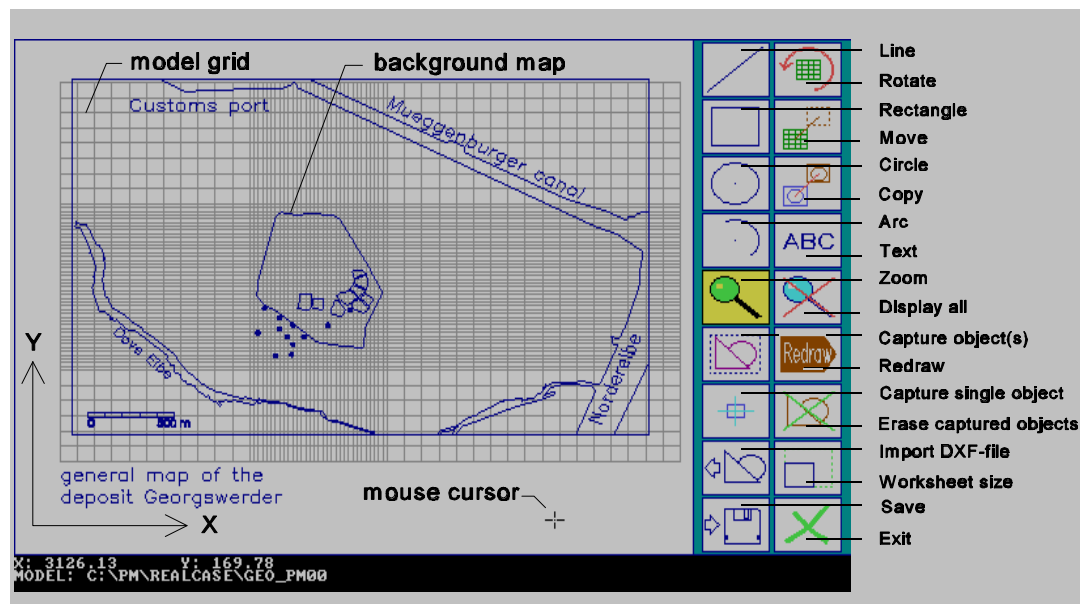
Fig. 4.1: The model worksheet and function buttons of PMCAD

You can use a function shown on the right-hand side of the screen only if it is activated and colored in yellow. To activate a function, just click the mouse cursor on the function button. The functions of PMCAD are described in the following:

- **Line**. Click the mouse cursor on the desired starting point of a line (i.e. move the mouse cursor to the desired starting point of a line and press the left mouse button once) and click the mouse cursor on the desired endpoint again. The endpoint will automatically be set as starting point of the next line. You can continue to draw the next line or press the right mouse button to stop the draw line function.
- **Rectangle**. Click the mouse cursor on the desired position of any corner of a rectangle, move the mouse cursor and click the mouse cursor on the opposite corner of the rectangle.
- **Circle.** Click the mouse cursor on the desired position of the circle's center, move the mouse cursor to draw the circle and press the left mouse button.
- **Arc**. Click the mouse cursor on the desired position of the center of an arc, click the mouse cursor on the desired starting position of the arc and move the mouse cursor to draw the arc. Note that an arc can only be drawn counterclockwise.
- **Rotate**. An object is captured by using the "capture object(s)" or "capture single object" functions described below. If a captured object is not present, the user can use this function to rotate the model grid. Otherwise, you can rotate the captured object(s) by clicking the mouse cursor on the rotation center and rotate the object(s) by moving the mouse.
- **Move**. If a captured object is not present, the user can use this function to move the model

grid. Otherwise, you can move the captured object(s) by clicking the mouse cursor on a base point and drag the object(s) to the desired location by using the mouse.

- **Copy.** This function is similar to the "Move grid/captured object(s)" function described above, but it puts copies of the captured objects at the specified location.
- **Text.** Click the mouse cursor on the starting point of a text. The left end of the text baseline will be placed on the starting point. Before the text can be drawn, the desired height, the rotation angle for the text and the text string itself must be specified. The unit for the height of the text string is the same as the length unit of the model.
- **Zoom**. Use this function to increase the apparent size of the model area, although the actual size remains constant. As the user increases the apparent size of the model area, the user views a smaller area of the model in greater detail. The "Zoom window" is specified by clicking the mouse cursor on the opposite corners of the window.
- **Display all.** Switches the model designer to display the entire model area.
- **Redraw**. Refreshes the map display on the model worksheet.
- **Capture object(s)**. An object is captured when the object is inside a "capture window". The "capture window" is specified by clicking the mouse cursor on the opposite corners of the window. To **unselect** the captured object(s), use the "capture window" again. Press the right mouse button to **unselect all** captured objects while the "Capture object(s)" function is currently being activated. A captured object is colored in light blue.
- **Capture single object**. Click the mouse cursor on an object which should be captured or unselected.
- **Erase captured object(s).** Click the mouse cursor on this button to erase the captured objects.
- **Worksheet size.** Click the mouse cursor on this button to change the size of the model worksheet by specifying the coordinate of the lower-left and the upper-right corners of the model worksheet.
- **Import DXF-file**. Up to three DXF-maps can be displayed simultaneously, but they cannot be modified in PMCAD. The DXF graphics entities LINE, POLYLINE, POINT, CIRCLE, ARC, and TEXT can be accepted. There is no size limit to the number of these graphics entities. The scale factor of a DXF-map and the displacement of a **scaled** DXF-map must be carefully specified in the "IMPORT DXF-FILE" dialog box (Fig. 4.2). A DXF-map will be displayed only if the option "DISPLAY" is chosen, i.e. an "X" in the square brackets. You can use this option to turn off the display of a DXF-map, without having to erase the filename given in the dialog box.

Important: If an incorrect scale factor or displacement is used, the DXF-map cannot be

displayed correctly. In many cases, a DXF-map with an incorrect scale factor or displace-
ment will be displayed too small, too large, or outside the model worksheet. If you are using
drawing programs, such as CorelDRAW or SURFER, to create DXF-maps, you should be
aware that a DXF-map can be rescaled by these programs.

- **Save.** Saves the map in the PMCAD- or DXF-format.
- **Exit.** Exits **PMCAD.**
- **[F12]-key**. press this key once to hide the model grid. To show the model grid press the key again. This function is not shown on the screen.
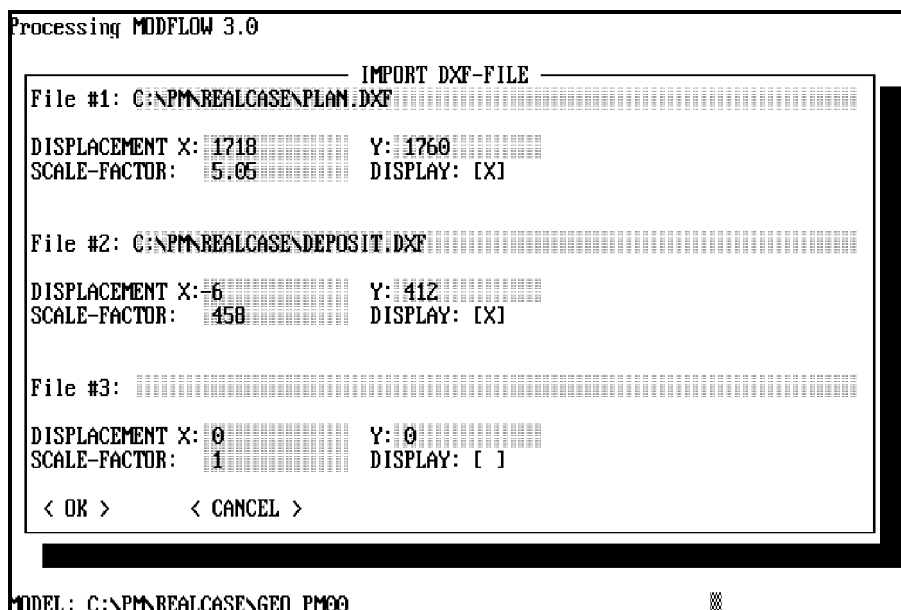
Fig. 4.2: Import DXF-file

4.1.2 The zones editor

The zones editor allows the user to specify the areally-distributed physical data in form of zones (Fig. 4.3). A zone consists of a series of connected nodes and connection lines. Each zone contains a value for the physical data currently being edited. A model cell will get the value of a zone when its center is inside the zone.

Through the use of the functions shown on the right-hand side of the screen, zones can be drawn or erased and values can be assigned to zones. The zonation data will be transferred to the model cells only when the "Transfer" function is used. To activate or use a function, click the mouse cursor on the function button. An activated function is colored in yellow. The use of the functions are described below:
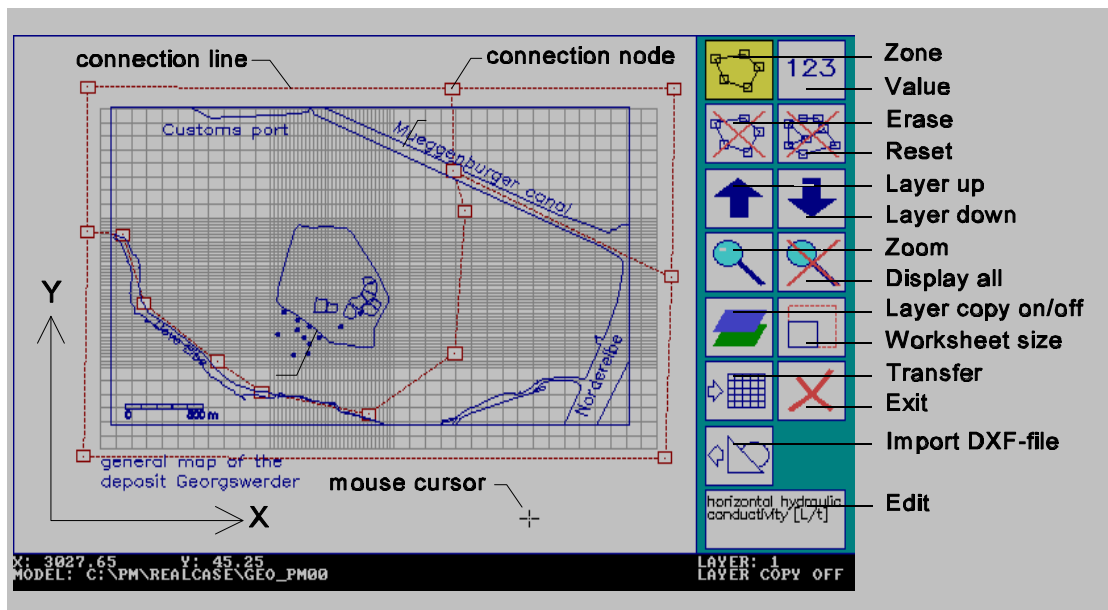
Fig. 4.3: Specification of zonation data with the zones-editor

- **Zone.** Draws a zone or a contour by clicking the mouse cursor on the desired position. The first and last connection node must overlap. The contours of the areally distributed data must be specified in order, from the innermost contour to the outermost contour. During the zone specification you can press the right mouse button to abort the input.
- **Value.** To assign a value to a zone, first move the mouse cursor to the inside of a zone (The boundary of this zone will be colored in yellow), click the mouse cursor once, then type the value at the prompt.
- **Erase.** To erase a contour or a zone, first move the mouse cursor to the inside of a zone then click the mouse cursor once.
- **Reset.** Deletes all zones or contours of the current layer.
- **Layer up.** Saves the data of the current layer and loads the data of the upper neighboring layer into the worksheet.
- **Layer down.** Saves the data of the current layer and loads the data of the lower neighboring layer into the model worksheet.
- **Zoom**. Use this function to increase the apparent size of the model area, although its actual size remains constant. As the user increases the apparent size of the model area, the user views a smaller area of the model in greater detail. The "Zoom window" is specified by clicking the mouse cursor on the opposite corners of the window.
- **Display all**. Switches the model designer to display the entire worksheet (see **Worksheet size** below).
- **Layer copy on/off.** Switches the layer copy function on or off. If the user turns on the "Layer copy" function, the model data of the current layer can be copied to an adjacent layer by using

the "Layer up" or "Layer down" function.

- **Worksheet size**. Click the mouse cursor on this button to change the size of the model worksheet by specifying the coordinates of the lower-left and the upper-right corners of the worksheet.

> Through the use of this function, the zonation data will be transferred to the model cells. The cell-by-cell data are actually used by <u>all</u> other programs of **PM**. Once the zonation data is transferred to the cells, you can use the cell-by-cell grid editor to change the data of each cell individually or use **PMGRAF** to make a graphic plot of the data.

- **Transfer.**
- **Exit.** Exits the zones editor.
- **Import DXF-file.** Allows the user to load and display up to three DXF-maps simultaneously. Please see section 4.1.1 for detailed information.
- **Edit.** A window shows the physical parameter currently being edited.

4.1.3 The grid editor

The cell-by-cell grid editor is designed to help the user specify or modify the data of each cell individually. While the model grid can be rotated in PMCAD, it will always be displayed parallel to the model worksheet of the grid editor. The background maps and the user-drawn map can be displayed by the grid editor (Fig. 4.4). However, the graphics outside of the model grid cannot be displayed, because the size of the worksheet cannot be changed within the grid editor.

The grid editor can be used for specifying data for various parameter types. The parameter type currently being edited will be shown in the information area of the Fig. 4.4 (e.g., Well [L^3/T] (+)recharge (-)discharge). If you are preparing data for a transient flow simulation, the current stress period number will also be shown in the information area, e.g, *stress period 1*. Because cells with different boundary conditions or values can be shaded with different colors, a legend is displayed in the information area.

The grid cursor can be moved by using the arrow keys or by clicking the mouse on the desired position. The cell value at the current position of the grid cursor will be shown in the status line and can be edited by using the functions shown in the right-hand side of Fig. 4.4. The position of the grid cursor specified by three indices for layer, x- and y-direction is shown in the status lines. In the grid editor, the x, y and z coordinate axes are oriented along the row, column and layer directions, respectively. The origin of the coordinate system is located at the upper, top, left corner of the cell at the first row, first column and first layer as illustrated in Fig. 4.5.
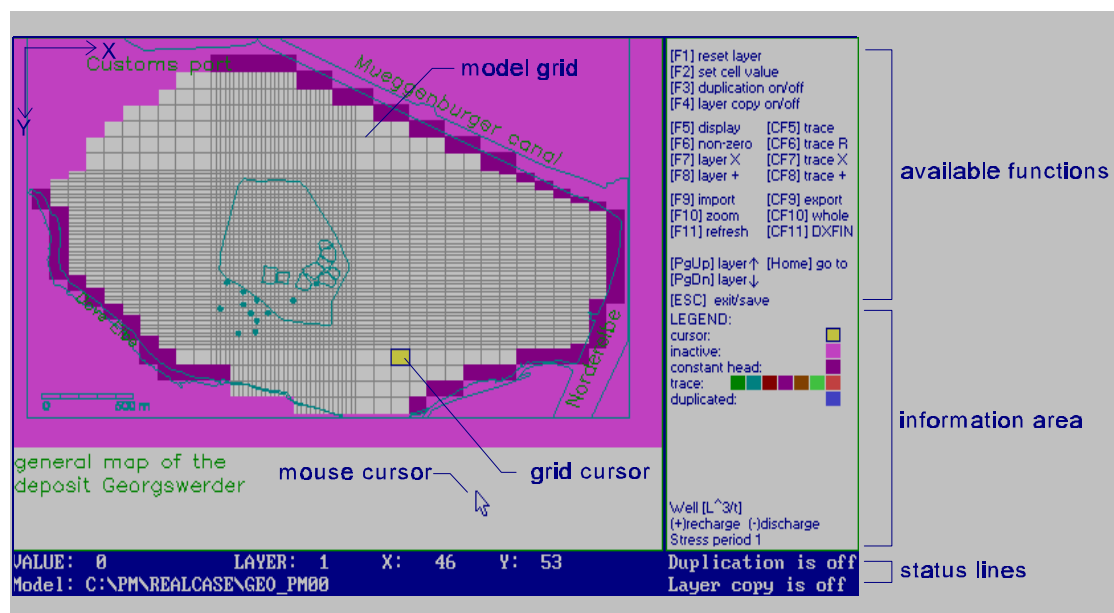
Fig. 4.4: The cell-by-cell grid editor
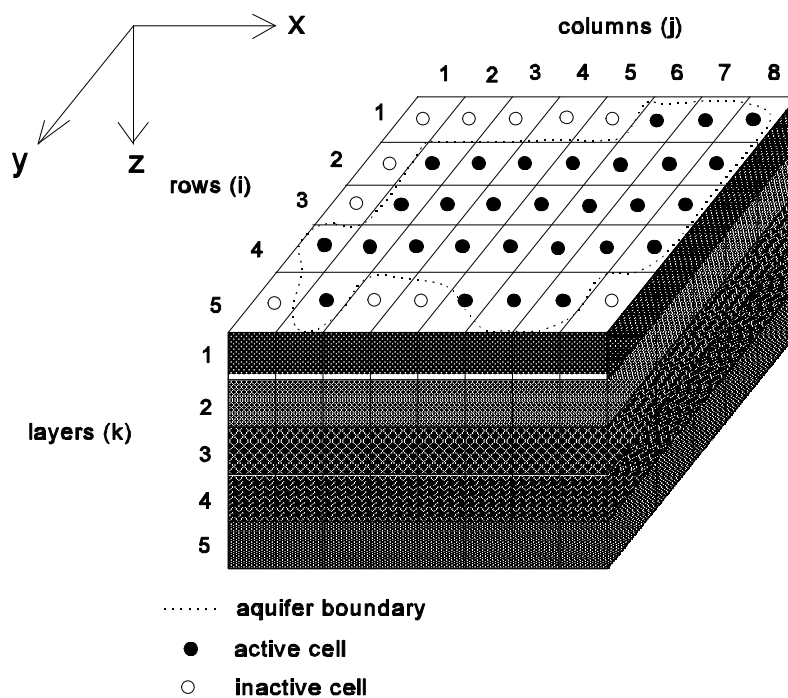
Fig. 4.5: Coordinate system used in the grid editor (after McDonald and Harbaugh, 1988)

The model data of each cell can be edited by using the function keys shown in the right-hand side of Fig. 4.4. The combination of the letter "C" and a function name means a key combination with the Ctrl key. For example, [CF5] means the key combination Ctrl+F5. The following list explains the use of these functions:

- **[F1] reset layer.** Set a constant value to all cells of the layer currently being edited.
- **[F2] set cell value.** Set a value to the cell at the current cursor position.
- **[F3] Duplication on/off**. Switches the duplication function on or off. If the user turns the function "Duplication" on, the cell value at the current cursor position can be copied to an adjacent cell by moving the grid cursor with the direction keys or the mouse.
- **[F4] Layer copy on/off**. Switches the layer copy function on or off. If the user turns on "Layer copy", the model data of the current layer can be copied to an adjacent layer by using the [PgUp] or [PgDn] function or to an other layer by using the [Home] function.
- **[F5] display.** Through the use of this function, the grid editor can be switched to display an irregularly spaced model grid in its actual size or in regularly spaced form. In the last case, the background maps will not be displayed.
- **[F6] non-zero.** Show the cells with a non-zero value.
- **[F7] layer ×.** Multiply all cell values of the current layer by an user-specified factor.
- **[F8] layer +.** Add a constant value to all cell values of the current layer.
- **[F9] import.** Reads a data array from a user-specified file into the current layer. (See Appendix E for the data structure)
- **[F10] zoom.** Use this function to display a "zoom area" in greater detail. This area is specified by clicking the mouse cursor on the opposite corners of a "zoom window".
- **[F11] refresh.** Redraw the model grid without changing the model data.
- **[CF5] trace.** Show all cells that have a value located between a minimum and a maximum specified by the user.
- **[CF6] trace R(eplace).** Show all cells that have a value located between a minimum and a maximum specified by the user and change these cell values to a user-specified value.
- **[CF7] trace ×.** Show all cells that have a value located between a minimum and a maximum specified by the user. These cell values will be multiplied by a user-specified factor.
- **[CF8] trace +.** Show all cells that have a value located between a minimum and a maximum specified by the user and add a user-specified constant to these values.
- **[CF9] export.** Save the model data of the current layer in an ASCII file. This file can be reloaded by using the import function [F9].
- **[CF10] whole.** Display the entire model grid.
- **[CF11] DXFIN.** Allows the user to load and display up to three DXF-maps simultaneously. Please see **Import DXF-file** in section 4.1.1 for detailed information.

- **[PgUp] layer ↑.** Saves the data of the current layer and moves the grid cursor to the upper neighboring layer. The model data of the current layer will be copied to the upper neighboring layer if "Layer copy" is turned on by using [F3].

- **[PgDn] layer ↓.** Saves the data of the current layer and moves the grid cursor to the lower neighboring layer. The model data of the current layer will be copied to the lower neighboring layer if "Layer copy" is turned on by using [F3].

- **[Home] go to.** Saves the data of the current layer and moves the grid cursor to a user-specified layer. The model data of the current layer will be copied to the destination layer if "Layer copy" is turned on by using [F3].

- **[ESC] Exit.** Exits the grid editor. If you have more than one stress period, an option box will come up which allows you to manage model data for a transient simulation (Fig. 4.6). If the model data for a stress period is not specified, the default value of zero will be used.
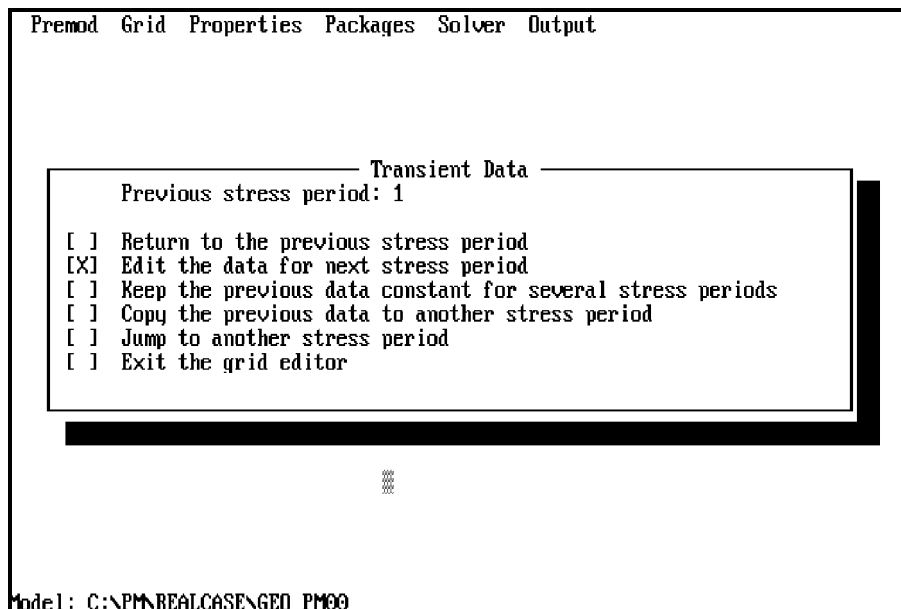
Fig. 4.6: Option box for editing of transient data

4.2 PREMOD - Preprocessor for MODFLOW/MODPATH

After having created or loaded a model and selected the menu item "Edit flow model" from the "Model" menu of the PM-shell, PREMOD (the preprocessor for MODFLOW) will be loaded. Like the PM-shell, PREMOD also uses pull-down menus. The menu bar of PREMOD contains six menu titles (Fig. 4.7). The "Premod" menu allows the specification of time parameters and the selection of a simulation type between steady-state and transient flow. Through the use of the "Grid" and "Properties" menus and the help of the model designer, you can specify the dimension of the model grid, initial and boundary conditions and the properties of the porous media, e.g., porosity or hydraulic conductivity. In MODFLOW, each package deals with a specific feature of the hydrologic system to be simulated, such as wells, recharge or river. You can activate or deactivate a package by using the "Package" menu. From the "Solver" menu, a specific method of solving a system of linear equations which describes the flow system can be selected. Use of the "Output" menu allows you to decide which simulation results to be saved or printed and when they should be saved or printed.

In the following sections, the use of each menu will be described in detail.
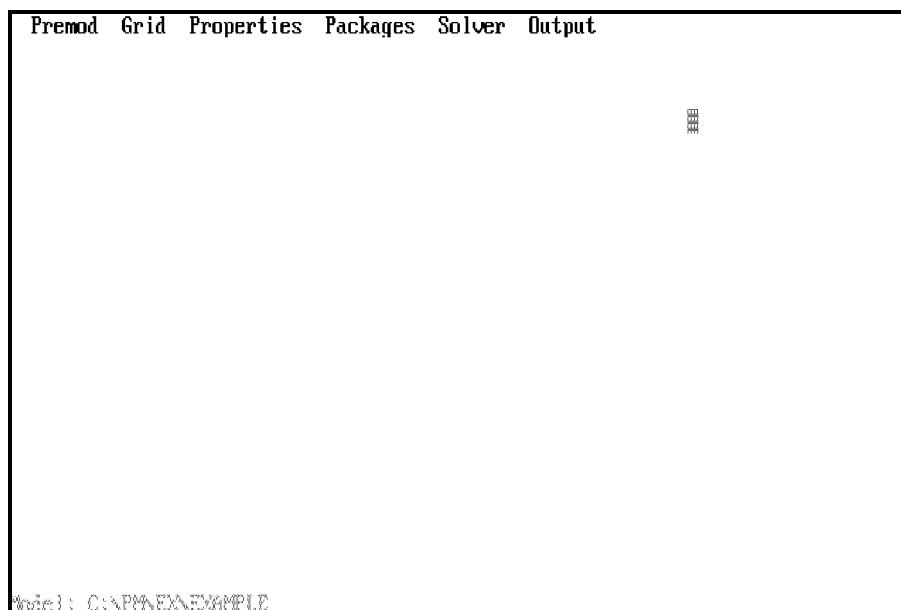
Fig. 4.7: Menu bar of PREMOD

4.2.1 The "Premod" menu

The "Premod" menu contains five menu items (Fig. 4.8), which are described below:

Fig. 4.8: The "Premod" menu

About Premod:
Shows general information about the preprocessor PREMOD.

Steady state:
To prepare model data for simulation of steady state groundwater flow, select this menu item. A dialog box will come up, and ask for a time unit (Fig. 4.9). Select a time unit by entering a number between 0 and 5 as indicated in the "Time units" box. Please note that this time unit is used for identification purposes only, it is not used in the simulation, and dose not affect the simulation results in any way. The time unit, which is actually used in the simulation, is given by the time unit of input variables (see p. 4-1).

After having selected a time unit, you will be asked to enter time parameters in a worksheet (Fig. 4.10). The worksheet contains four columns and as many rows as the number of stress periods (for simulation of steady flow, only one stress period is used). The meaning of each column title and the available command keys for editing the time parameters are given at the bottom of the worksheet. The worksheet allows a minimum value of -9.99E+29 and a maximum value of 9.99E+29. A seven-digits precision can be handled by the worksheet. If a precision greater than seven digits is used for data-entry, the worksheet may display the value incorrectly.

```
 Premod  Grid  Properties  Packages  Solver  Output

        Simulation parameters:

        Time unit of model data:    1


                < OK >                < CANCEL >




                                 ▓


                    ────────────── Time units ──────────────
                    0 - undefined   1 - seconds   2 - minutes
                    3 - hours       4 - days      5 - years
                    ──────────────────────────────────────────

 Model: C:\PM\EX\EXAMPLE
```

Fig. 4.9: Selection of a time unit

```
PREMOD: Simulation time (Steady State)
┌─────────┬──────────┬─────────┬─────────┬──────────────────┐
│ PERIOD  │  PERLEN  │   NSTP  │  TSMULT │                  │
├─────────┼──────────┼─────────┼─────────┤                  │
│       1 │ 3.14E+07 │       1 │       1 │                  │
│         │          │         │         │                  │
│         │          │         │         │                  │
│         │          │         │         │                  │
│         │          │         │         │                  │
│         │          │         │         │                  │
│         │          │         │         │                  │
└─────────┴──────────┴─────────┴─────────┴──────────────────┘
<ENTER>:EDIT  <ESC>:CANCEL  <Alt-Z>:SAVE/EXIT  <PgUp> <PgDn> ↑ ↓ ← →

PERIOD is the stress period
PERLEN is the length of stress periods
NSTP is the number of time steps within a stress period
TSMULT is the multiplier for length of time steps



 Model: C:\PM\EX\EXAMPLE
```

Fig. 4.10:   Specification of time parameters for the simulation of steady flow

The following command keys can be used within the worksheet:

Arrow keys: Move the worksheet pointer in the direction of the arrows to highlight a value.

PgUp/PgDn: if more than 10 stress periods are required (for a transient flow simulation), these keys can be used to move cursor up or down 10 stress periods.

ENTER: to edit a value, move the pointer to the value, type in the new value and then press the ENTER key.

ESC: allows you to abandon the changes you have made.

Alt-Z: you can save the changes and leave the worksheet by holding down the Alt key and pressing "Z".

In MODFLOW, the simulation time is divided into stress periods - time interval during which all external stresses are constant - which are, in turn, divided into time steps. For simulation of steady flow, the number of time steps within a stress period and the multiplier for the length of successive time steps should be equal to 1. The length of the stress period is important if you intend to do a transport simulation with MT3D.

Transient:

For the simulation of transient groundwater flow, select the menu item "Transient". A dialog box will come up and ask for the number of stress periods and for a time unit (Fig. 4.11). Select a time unit by entering a number between 0 and 5 as indicated in the "Time units" box. Like **Steady state**, this time unit is used for identification purposes only. After entering the number of stress periods and selecting a time unit, you will be asked to enter time parameters for each period in the worksheet shown in Fig. 4.12. The use of the worksheet is the same as described above. In the case shown in Fig. 4.11 and Fig. 4.12, a time unit of SECONDS and five stress periods are specified. The length of the first stress period is 3.14E+07 seconds (1 year), the other stress periods have a length equal to 6.28E+07 seconds. All stress periods are divided in one time step.
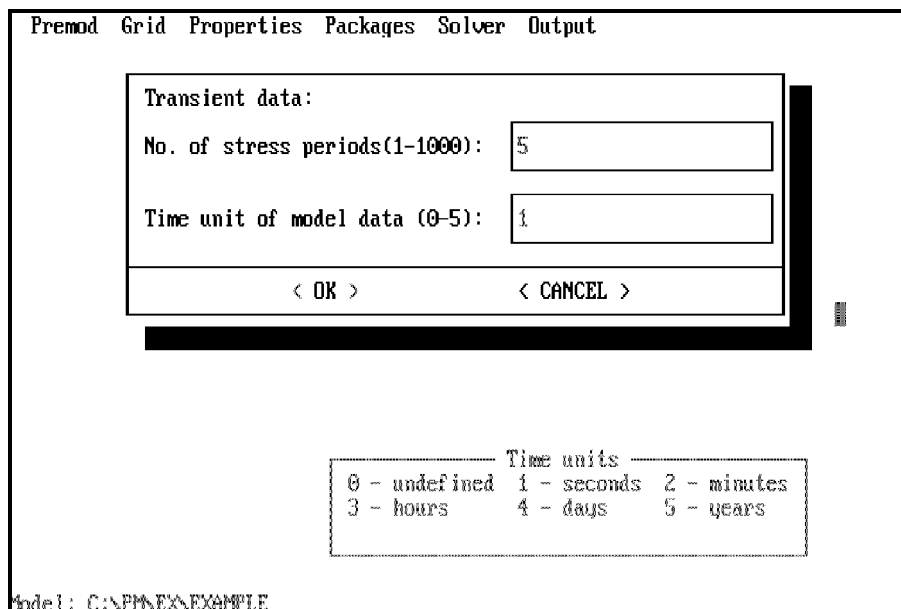
Fig. 4.11: Specification of the number of stress periods and selection of a time unit

```
┌─────────────────────────────────────────────────────────────┐
│PREMOD: Simulation time (Transient)                          │
│┌──────┬─────────┬─────────┬─────────┬─────────────────────┐ │
││PERIOD│  PERLEN │    NSTP │  TSMULT │                     │ │
│├──────┼─────────┼─────────┼─────────┤                     │ │
││     1│ 3.14E+07│       1 │       1 │                     │ │
││     2│ 6.28E+07│       1 │       1 │                     │ │
││     3│ 6.28E+07│       1 │       1 │                     │ │
││     4│ 6.28E+07│       1 │       1 │                     │ │
││     5│ 6.28E+07│       1 │       1 │                     │ │
││      │         │         │         │                     │ │
││      │         │         │         │                     │ │
││      │         │         │         │                     │ │
││      │         │         │         │                     │ │
││      │         │         │         │                     │ │
│└──────┴─────────┴─────────┴─────────┴─────────────────────┘ │
│<ENTER>:EDIT <ESC>:CANCEL <CTRL-END>:SAVE/EXIT <PGUP> <PGDN> ↑ ↓ ← →│
│                                                             │
│PERIOD is the stress period                                  │
│PERLEN is the length of stress periods                       │
│NSTP is the number of time steps within a stress period      │
│TSMULT is the multiplier for length of time steps            │
│                                                             │
│                                                             │
│Model: C:\PM\EX\EXAMPLE                                      │
└─────────────────────────────────────────────────────────────┘
```

Fig. 4.12:   Time parameters for the simulation of transient flow

Transfer model data:

To reduce the processing time, PREMOD internally saves model data in binary files. Through a translator, these binary files will be converted into ASCII files, which are actually used by MODFLOW, MODPATH and MODPATH-PLOT. The translator is called by selecting the menu item "Transfer model data". If the color of this menu item is gray, the translator will not be loaded and the computer will beep. This means that the model data is not complete. You must check whether you have forgotten to specify some model data, to select a solver or something else.

> **Please note that "Transfer model data" must be performed whenever you have made changes in your model. Otherwise, the ASCII model files will not be modified.**

Exit:

To exit PREMOD and return to the PM-shell, select this menu item.

4.2.2 The "Grid" menu

The "Grid" menu contains eight menu items (Fig. 4.13). The menu item "WETDRY (wetting capability)" appears only when you have installed **PM** to run with the BCF2 Package of MOD-FLOW. The symbol » shown in the front of a menu item indicates whether the data has been specified or not. If you are creating a new model, you must first specify the dimension of your model. This is done by selecting the menu items "X and Dx of cells (DELR array)", "Y and Dy of cells (DELC array)" and "Z of layers (TOP/BOT array)". Before you have specified the dimension of the model, the other menu items are colored in

gray and cannot be used.
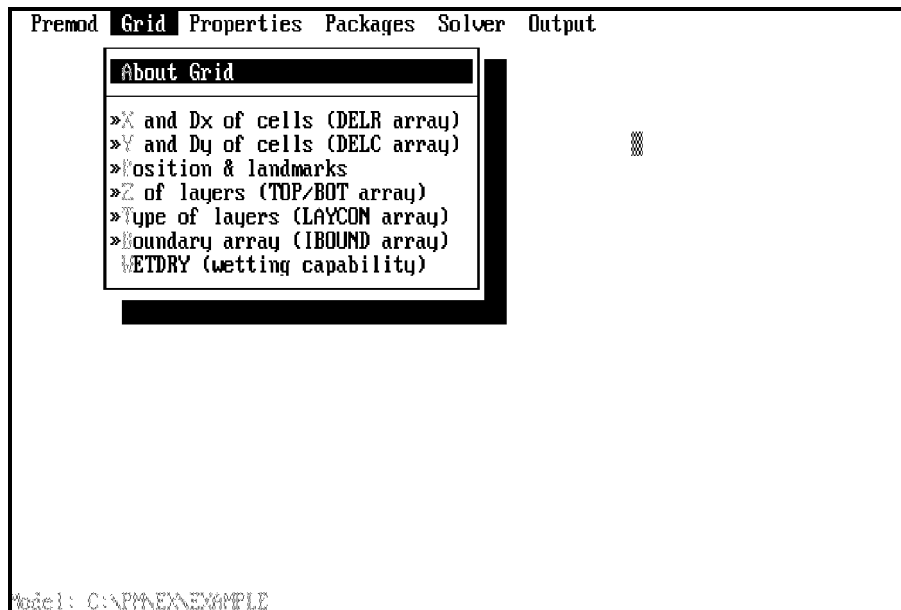
Fig. 4.13: The "Grid" menu

The menu items of the "Grid" menu are described below:

About Grid:
Shows general information about the "Grid" menu.

X and Dx of cells (DELR array):
To specify the number of cells and the cell width in the x-direction (along rows), select this menu item. If the number of cells in the x-direction has not been set, a dialog box will come up and ask for the number of cells and a length for all cells in the x-direction (Fig. 4.14). The maximun number of cells in the x- or y-direction is 500 and a model layer can have up to 15000 cells. If you have 60 cells in the x-direction, then the maximum number of cells in the y-direction would be 250 (60×250=15000).

After having specified these data and selected "OK", the grid editor will come up (Fig. 4.15). You may notice that a lot of functions are not shown on the right-hand side of the screen. This is because they are not necessary for the specification of the cell sizes. The available functions of the grid editor will be used to change the cell width along rows. If you have an irregularly spaced model grid, the cell sizes shown on the screen will automatically be changed by the grid editor (Fig. 4.16). This can help you to visually control the cell width.
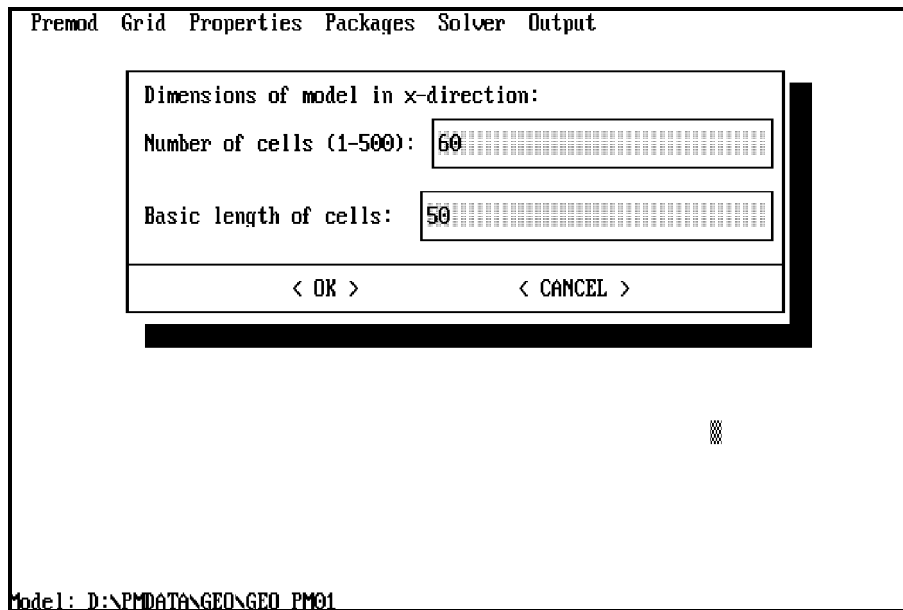
Fig. 4.14:   Specification of the number of cells and the basic length
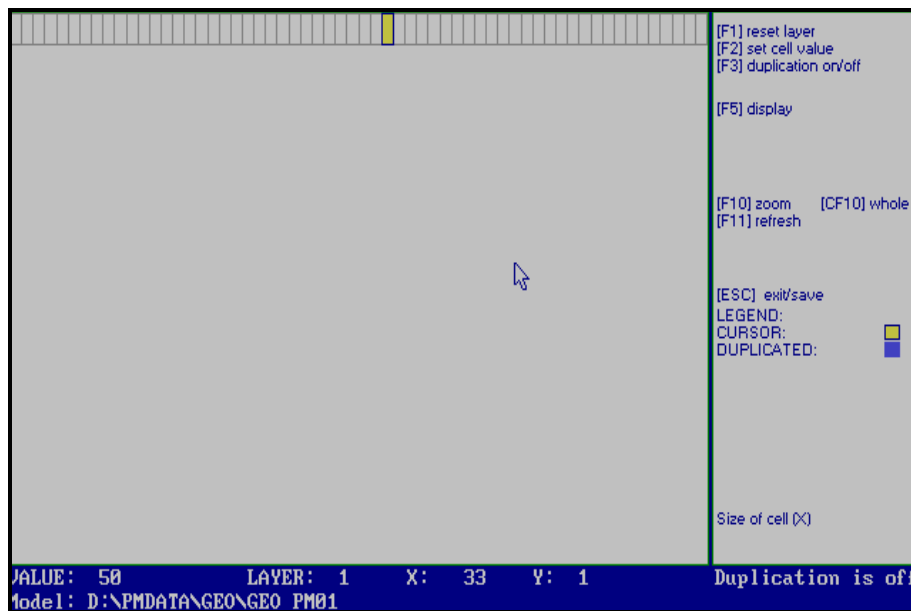
Fig. 4.15: Specification of the cell width along rows
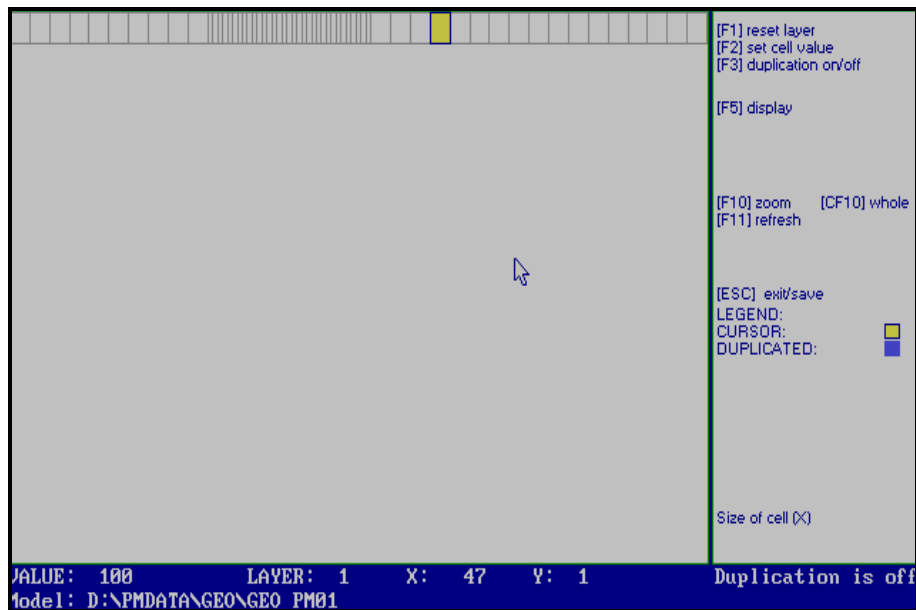
Fig. 4.16: Entry of an irregularly spaced model grid

Y and Dy of cells (DELC array):

To specify the number of cells and the cell width in the y-direction (along columns), select this menu item. If the number of cells in the y-direction has not been set, a dialog box will come up and ask for the number of cells and a length for all cells in the y-direction (Fig. 4.17). After having specified this data and selected "OK", the grid editor will come up. Like **X and Dx of cells**, you can use the grid editor to change the cell width along columns (Fig. 4.18).
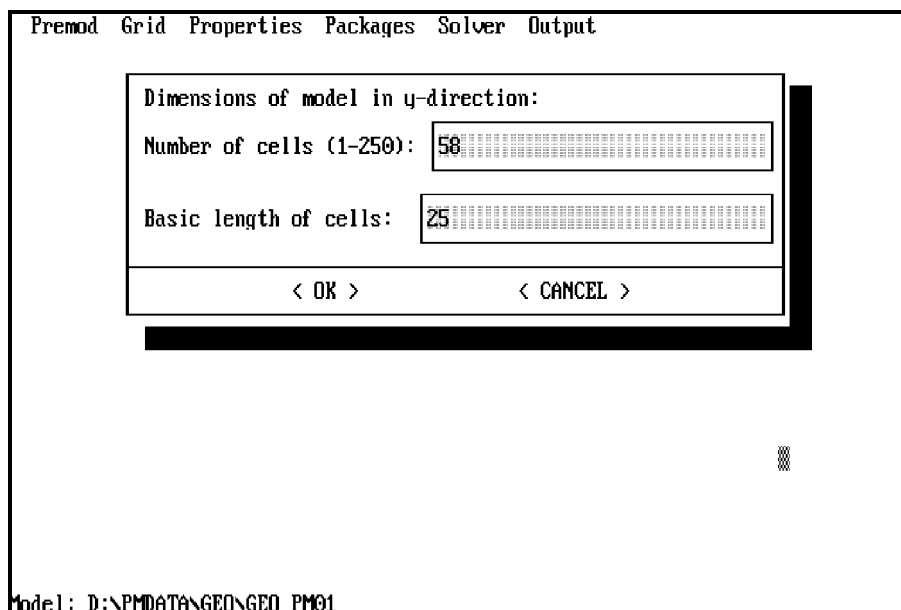
Fig. 4.17:   Specification of the number of cells and the basic cell length
                  in the y-direction
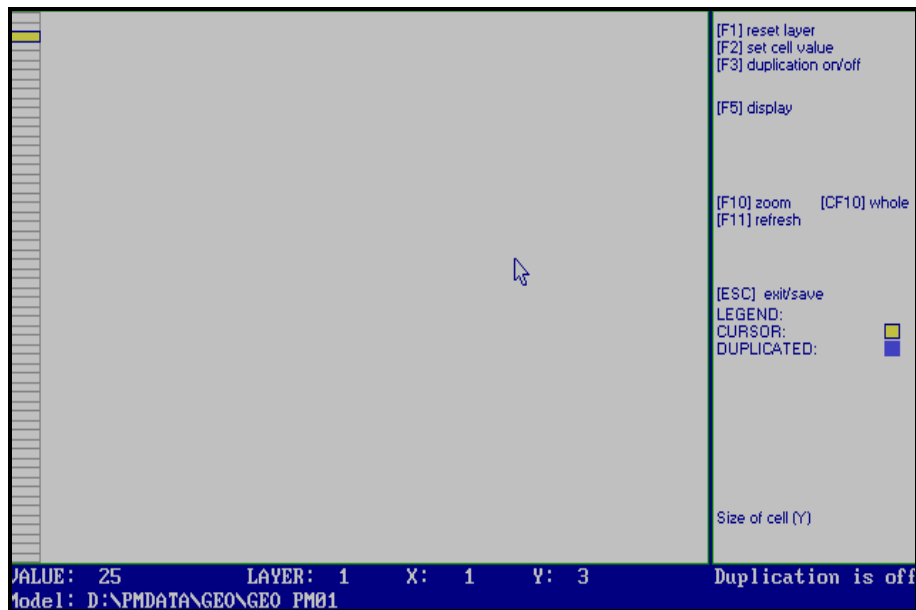
Fig. 4.18: Specification of the cell width along columns

Position & landmarks

Select the menu item "Position & landmarks" from the "Grid" menu to construct a general map of your model area. If you have created a new model, the model grid will be shown in the lower-left corner of the model worksheet (Fig. 4.19). By default, the origin of the coordinate system is set at the lower-left corner of the worksheet. The size of the worksheet is automatically set to fit the model grid. PMCAD allows you to display up to three DXF-background maps and a user-drawn map simultaneously. For detailed information about the use of PMCAD, please refer to section 4.1.1.
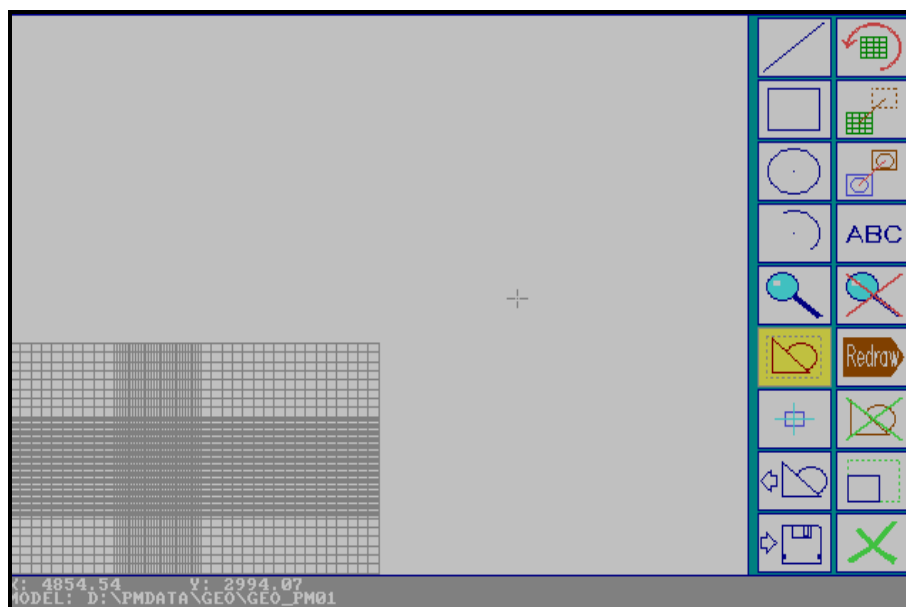
Fig. 4.19: The model grid and the default size of the worksheet

Z of layers

To specify the elevation of layer top and layer bottom, select menu item "Z of layers (TOP and BOT array)" from the "Grid" menu. If the number of layers has not been set, a dialog box will come up (Fig. 4.20). After having specified the number of layers, you can choose a data specification method from another dialog box (Fig. 4.21). The zones editor will be called by selecting "zones & contours" and the grid editor by selecting "cell-by-cell". You will first be asked to specify the elevation of the layer top. After having saved the data by pressing the [ESC] key, PREMOD will ask you whether or not the elevation of the layer bottom should be set equal to the elevation of the top of the layer located immediately below. If this is true, answer YES to the prompt "Set bottom of layer automatically". After this, you can continue to specify the elevation of layer bottoms. Note that the elevation of the lowest layer bottom cannot be obtained from the layer top and therefore must be specified by the user. If it has not been specified, the default value of zero will be used.
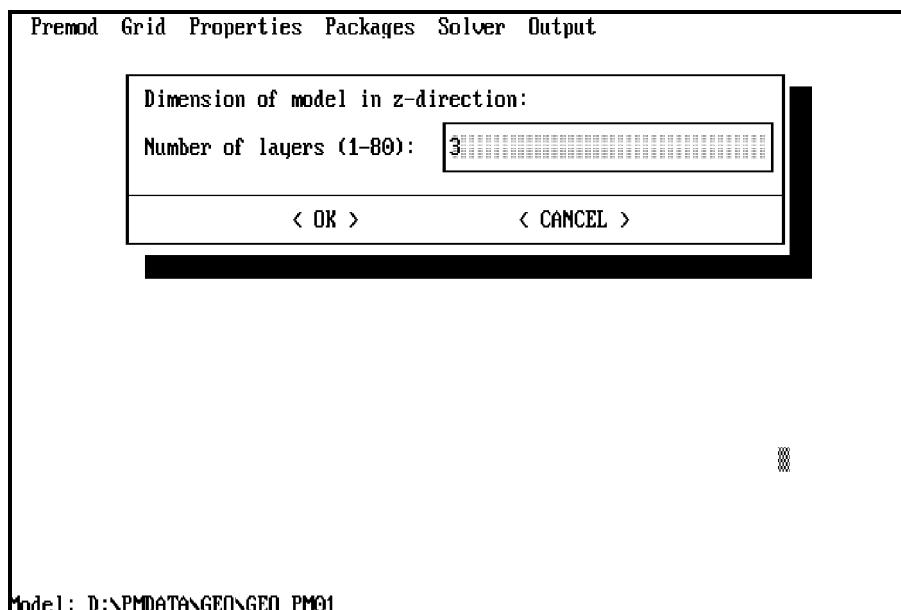
Fig. 4.20: Specification of the number of layers

```
 Premod  Grid  Properties  Packages  Solver  Output



              Select a data specification method

           < zones & contours >   < cell-by-cell >   < CANCEL >




Model: D:\PMDATA\GEO\GEO PM01
```
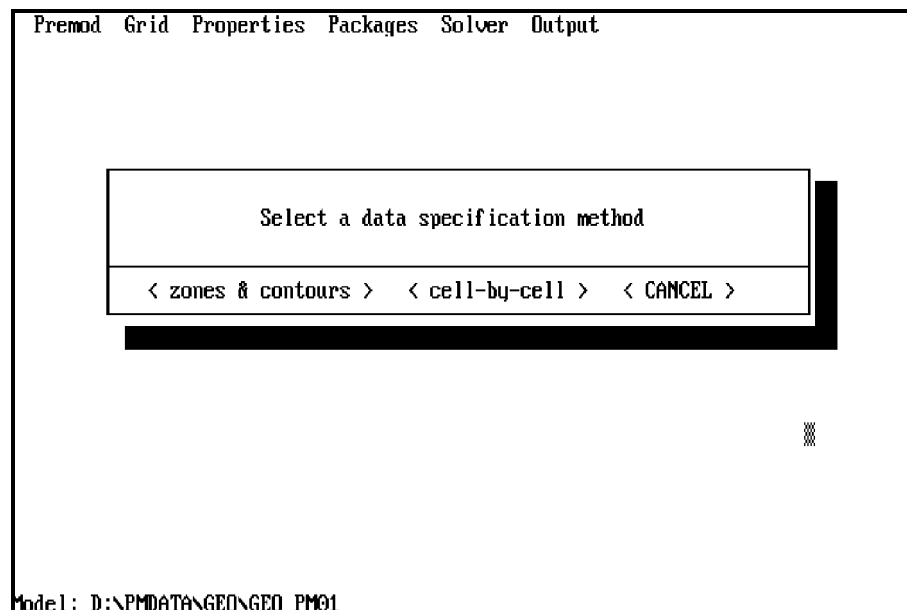
Fig. 4.21: Selection of a data specification method

Type of layers (LAYCON array)

To specify layer-type code and anisotropy factor for each layer, select the menu item "Type of layers (LAYCON array)" from the "Grid" menu. A dialog box will come up (Fig. 4.22).

```
 Premod  Grid  Properties  Packages  Solver  Output

      Layer: 1

      Layer type:      [0]

      Anisotropy factor(Tyy/Txx):   [1]

             < OK >               < CANCEL >


                     Type of Layers
         0 : confined
         1 : unconfined
         2 : confined/unconfined (Transmissivity constant)
         3 : confined/unconfined.
         4 - 7 : a quasi-3D confining layer is associated
                 with model layer of type 0 - 3

Model: D:\PMDATA\GEO\GEO PM01
```
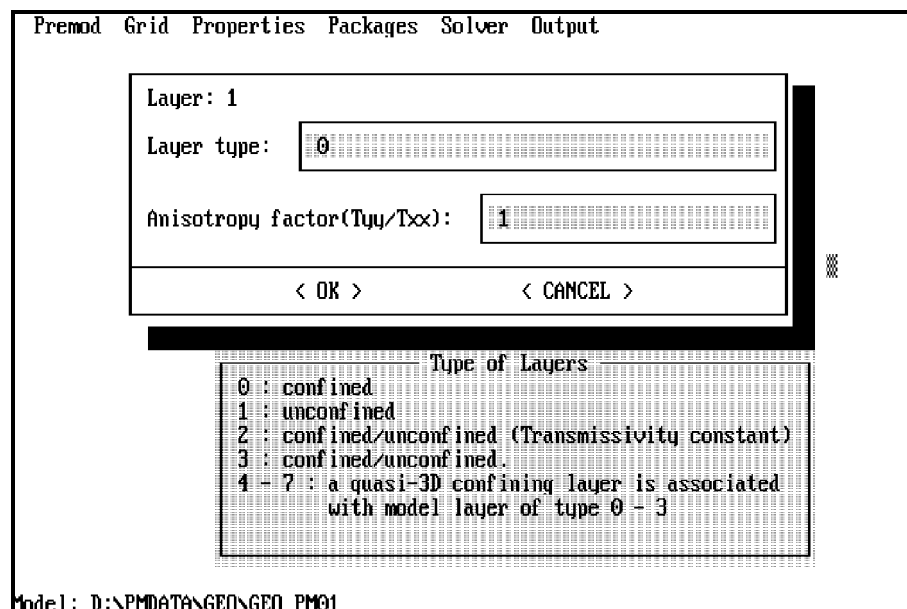
Fig. 4.22: Layer-type code and the anisotropy factor

The anisotropy factor is the ratio of transmissivity or hydraulic conductivity (whichever is being used) along the y-direction to the transmissivity or hydraulic conductivity along the x-direction. This factor is equal to 1.0 for isotropic conditions. MODFLOW can only consider horizontal anisotropy. The principal axes of the conductivity tensor must be parallel to the x- and y-axes of

your model grid.

The numerical formulations, which are used by the BCF-package to describe groundwater flow, depend on the "layer-type code" of each model layer. The codes are described below:

0: confined. The layer is strictly confined. For transient simulations, the storage coefficient is used to calculate the rate of change in storage. Transmissivity of each cell is constant throughout the simulation.

1: unconfined. The layer is strictly unconfined. This option is valid for layer 1 only. Transmissivity varies with the saturated thickness of the aquifer. The storage coefficient is constant.

2: confined/unconfined (Transmissivity constant). The layer type is partially convertible between confined and unconfined. Transmissivity is constant throughout the simulation. The storage coefficient may alternate between confined and unconfined values. Vertical leakage from above is limited at unconfined cells.

3: confined/unconfined. Fully convertible between confined and unconfined. Transmissivity of the layer varies with the saturated thickness of the aquifer. The storage coefficient may alternate between confined and unconfined values. Vertical leakage from above is limited at unconfined cells.

4: layer of type 0 to which a quasi-3D confining layer is associated.

5: layer of type 1 to which a quasi-3D confining layer is associated.

6: layer of type 2 to which a quasi-3D confining layer is associated.

7: layer of type 3 to which a quasi-3D confining layer is associated.

The last four types are only important if you want to compute pathlines in MODPATH for aquifer layers which are separated by semiconfining units (top of lower layer i   bottom of upper layer i-1). In MODPATH, each unsimulated confining layer is assumed to be part of the active model layer directly above it. It is assumed that one-dimensional, steady state vertical flow exists throughout the confining layer. This assumption implies that the average vertical linear velocity is constant throughout the confining layer and that its magnitude equals the volumetric flow rate between adjacent model layers divided by the horizontal area of the cell and the porosity of the confining layer. In **PM**, the porosity of the confining layer is assumed to be the same as the porosity of the layer directly above the confining layer.

Boundary array (IBOUND array)

The IBOUND array contains a code for each cell indicating whether (1) the head varies with time (active variable-head cell), (2) the head is constant (constant-head cell) or (3) no flow takes place within the cell (inactive cell). This array can be specified by using the zones editor or the grid editor. It is suggested to use 1 for an active cell, -1 for a constant head cell and 0 for an inactive cell.

WETDRY (wetting capability)

The menu item "WETDRY (wetting capability)" is shown only if you have installed PM to use the BCF2 Package of MODFLOW. The BCF2 Package makes it possible to simulate situations where the water table rises into unsaturated model layers. To use the wetting capability of the BCF2 Package, select the menu item "WETDRY (wetting capability)" and specify the parameters in a dialog box (Fig. 4.23). For explanations of the parameters, the equations 3a and 3b, the numerical formulations and the use of the wetting capability, please refer to the program documentation of the BCF2 Package (McDonald et al., 1991).

A WETDRY array is required for the wetting capability in addition to the parameters specified in Fig. 4.23. WETDRY is a combination of the wetting threshold (THRESH) and a flag indicating which neighboring cells can cause a cell to become wet. If WETDRY < 0, only the cell below a dry cell can cause the cell to become wet. If WETDRY > 0, the cell below a dry cell and the four horizontally adjacent cells can cause a cell to become wet. If WETDRY is 0, the cell cannot be wetted. When the sum of the BOT (elevation of the cell bottom) and the absolute value of WETDRY at a dry cell is equalled or exceeded by the head at an adjacent cell, the cell is wetted. Although the WETDRY is needed only for the layer of the type 1 or 3, it can be specified for all layers by using the zones editor or the grid editor. The wetting capability can be turned off by selecting the menu item "WETDRY (wetting capability)" again. Whether the wetting capability is activated or not is indicated by the symbol » in the front of the menu item.

```
 Premod  Grid  Properties  Packages  Solver  Output


            ┌──────── WETDRY OPTIONS ────────┐
            │                                │
            │ WETFCT factor: 0.1             │
            │                                │
            │ Iteration interval for attempting to wet cell:  1  │
            │                                │
            │ Select an equation used to calculate initial head at │
            │ cells that become wet:         │
            │                                │
            │ [X] (3a) h=BOT + WETFCT (hn - BOT) │
            │ [ ] (3b) h=BOT + WETFCT (THRESH)   │
            │                                │
            ├────────────────────────────────┤
            │   < OK >          < CANCEL >   │
            └────────────────────────────────┘



Model: D:\PMDATA\GEO\GEO_PM01
```
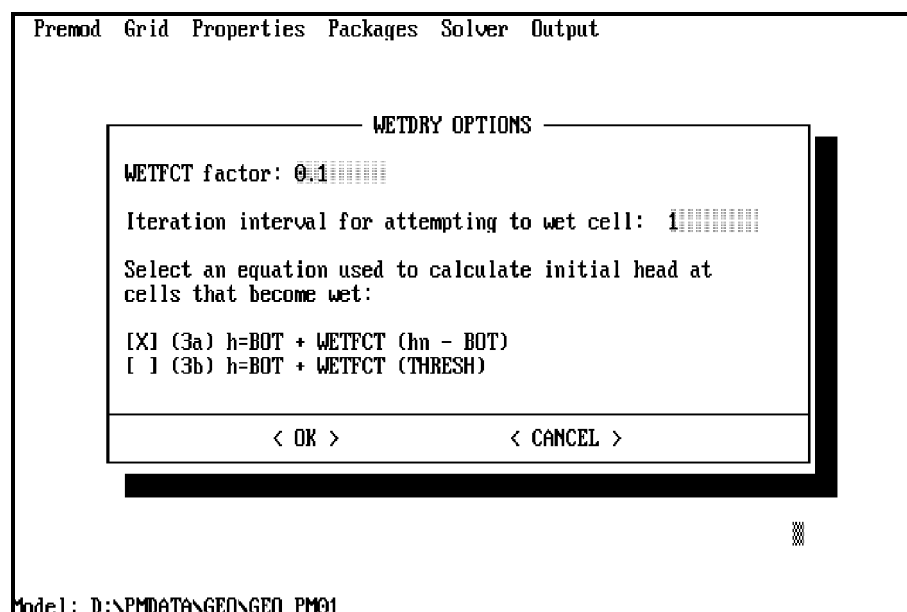
Fig. 4.23: Parameters for the wetting capability

4.2.3 The "Properties" menu

For the simulation of groundwater flow, the aquifer parameters must be specified. These parameters are porosity, specific storage, horizontal hydraulic conductivity, vertical hydraulic conductivity or vertical leakance and the initial hydraulic heads. They can be specified by using the zones editor or the grid editor. To edit a parameter, select the corresponding menu item from the "Properties" menu (Fig. 4.24). The symbol » shown in the front of a menu item indicates whether the data has been specified or not. If you have a steady state flow model, the menu item "Specific storage" is colored in gray. This means that the specific storage does not need to be input. The following paragraphs describe the use of each of the menu items.
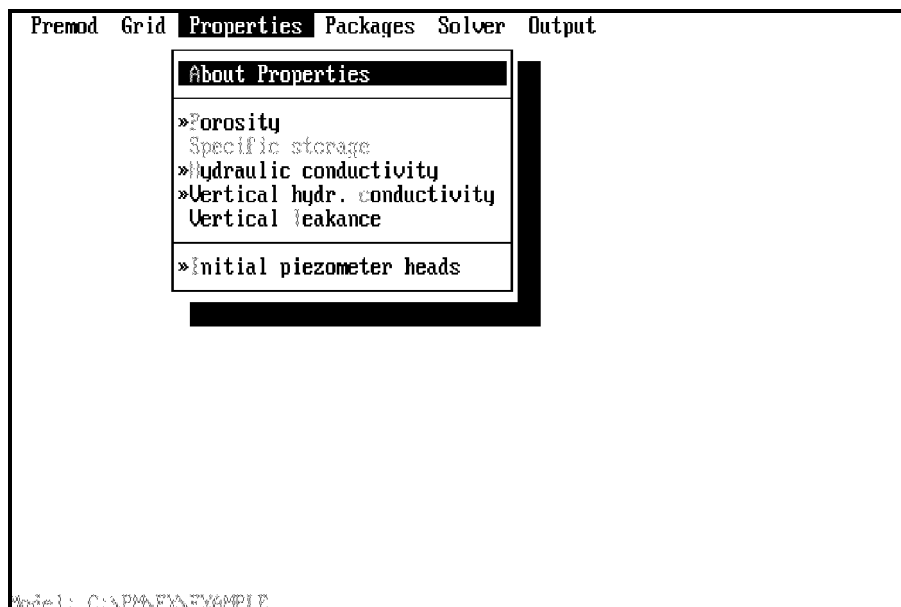
Fig. 4.24: The "Properties" menu

About Properties
Shows general information about the "Properties" menu.

Porosity
For the simulation of steady state flow, porosity (specific yield) is not required by MODFLOW. However, porosity is required by MODPATH for the calculation of the flow velocities and, therefore, this parameter must always be specified.

Specific storage
Although the input to the Block-Centered Flow (BCF) Package requires dimensionless storage coefficient values in each layer of the model, you only need to specify specific storage (dimension: L^{-1}) in PREMOD. The dimensionless storage coefficient is given by the specific storage of

the cell material multiplied by the layer thickness in the cell. PREMOD will take over the calculation of the storage coefficient.

Hydraulic conductivity

To specify horizontal hydraulic conductivity, select this menu item. If you have studied the input instructions of the BCF package of MODFLOW, you will notice that MODFLOW requires transmissivity for layers of type 0 or 2. For your convenience, PREMOD will take over the calculation of the transmissivity.

Vertical hydraulic conductivity and vertical leakance:

To calculate the vertical groundwater flow terms, MODFLOW needs an input data set of "vertical leakance". If you have a single-layer model, these menu items will be colored in gray and the input of these terms is not necessary. The term "vertical leakance" is defined in the BCF Package of the program documentation of MODFLOW (McDonald et al., 1988). In PREMOD, there are two ways to specify the vertical leakance:

1. Select the menu item "Vertical hydraulic conductivity" from the "Properties" menu. The vertical hydraulic conductivity of each cell is specified by the user. PREMOD calculates the vertical leakance with the equation:

$$\frac{1}{L} = \frac{d_1/2}{k_{fv,1}} + \frac{d_2/2}{k_{fv,2}}$$

where
L : vertical leakance
$k_{fv,1}$: *vertical hydraulic conductivity of the upper aquifer*
$k_{fv,2}$: *vertical hydraulic conductivity of the lower aquifer*
d_1 : *thickness of the upper aquifer*
d_2 : *thickness of the lower aquifer*
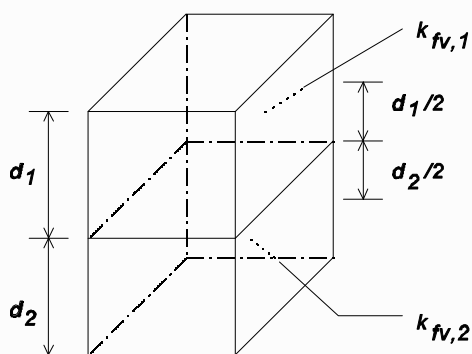
2. Select the menu item "Vertical leakance" from the "Properties" menu. The vertical leakance

is directly specified by the user. The following figure shows a situation where two layers are separated by a semiconfining unit (it is called "quasi-3D confining layer" by MODPATH). In this case, the vertical leakance is:

$$\frac{1}{L} = \frac{d_1/2}{k_{fv,1}} + \frac{d_2/2}{k_{fv,2}} + \frac{d_c}{k_{fv,c}}$$

where
L : vertical leakance
d_1 : thickness of the upper aquifer
d_2 : thichness of the lower aquifer
d_c : thickness of the semiconfining layer
$k_{fv,1}$: vertical hydraulic conductivity of the upper aquifer
$k_{fv,2}$: vertical hydraulic conductivity of the lower aquifer
$k_{fv,c}$: vertical hydraulic conductivity of semiconfining layer
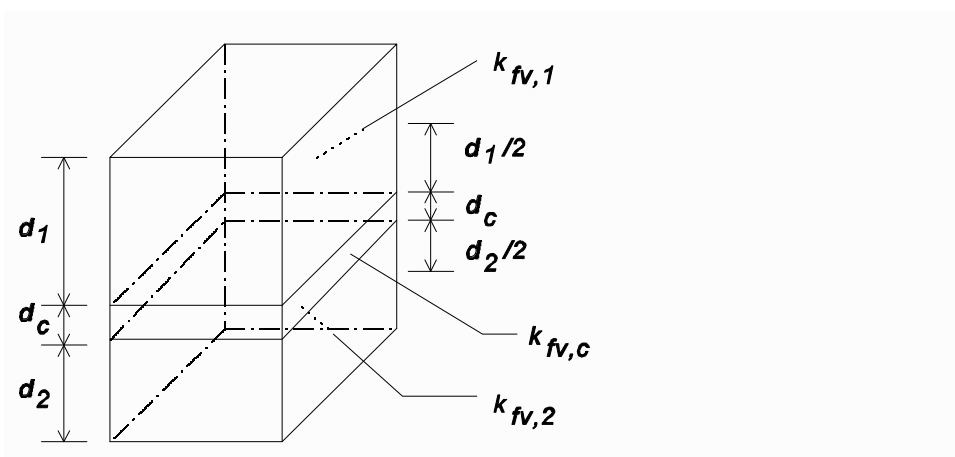
Initial piezometer heads

The initial hydraulic heads are heads at the beginning of the simulation. In many cases, the hydraulic heads will be obtained from a previous model run. The data import capability of the grid editor allows you to read these heads into the model grid. For more information, please refer to Appendices E and F.

4.2.4 The "Packages" menu

The user may activate the following stress packages by selecting the corresponding menu item from the "Packages" menu (Fig. 4.25):

Well Package (WEL1)
Drainage Package (DRN1)
River Package (RIV1)
Evapotranspiration Package (EVT1)
General-Head Boundary Package (GHB1)
Recharge Package (RCH1)
Stream-aquifer relation Package (STR1)

Fig. 4.25: The "Packages" menu

If an activated package is no longer necessary for a simulation, it can be switched off by selecting the corresponding menu item again. Whether a package is activated or not is indicated by the symbol » in front of the menu item. The data of a package will not be lost by switching it off. That is, when you switch it on again, the data which you have entered will automatically be reloaded. Unlike the areally distributed data, which can be specified by using the zones editor, the package data can only be specified by using the grid editor. The following paragraphs describe each of the menu items.

About Packages
Describes the basic use of the "Packages" menu.

Well

After selecting the menu item "Well" from the "Packages" menu, the grid editor will come up. The abstraction rate of a well is defined by a negative cell value and the injection rate by a positive cell value.

Drain

To simulate the effects of drains, two data sets are required:
- hydraulic conductance $[L^2/T]$ of the interface between the aquifer cell and the drain
- elevation of the drain [L].

After selecting the menu item "Drainage", the grid editor will come up and ask for the hydraulic conductance, as indicated by the appearance of "hydraulic conductance [L^2/T]" in the information area of the right-hand window (Fig. 4.26). The hydraulic conductance (CDRN) of the interface between the aquifer and the drain is given by:

$CDRN = K \times L$

where:

   K: hydraulic conductivity of the interface material [L/T]

   L: length of the drain in the cell [L]
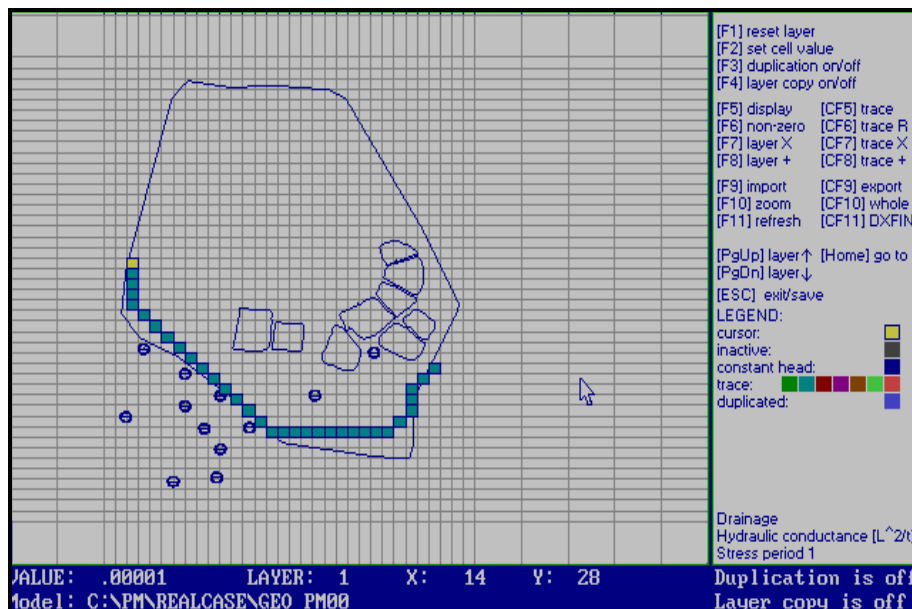
Fig. 4.26: Specifying the hydraulic conductance of drains

A non-zero hydraulic conductance for a cell indicates that it is a drain cell. After having saved the hydraulic conductance by pressing the [ESC] key, the grid editor will ask for the elevation of the drain by showing the message "Elevation of the drain" in the information area. The drain cells will

be colored in light blue. This helps the user to locate the exact position of the drain cells.

River

The purpose of the River Package is to simulate the effects of flow between surface-water features and groundwater systems. To simulate these effects, three data types are required for each river cell:

- hydraulic conductance of the riverbed [L^2/T]

- elevation of the riverbed bottom [L].

- head in the river [L]

The grid editor will ask for the data by showing a corresponding message in the information area. The process for specifying data into the River Package is similar to that of the Drain Package.

The hydraulic conductance of the riverbed (CRIV) is given by

$\quad$ CRIV = K $\times$ L $\times$ W / M

$\quad$ where:

$\quad\quad$ K: riverbed hydraulic conductivity [L/T]

$\quad\quad$ L: length of the reach contained in the river cell [L]

$\quad\quad$ W: width of the river [L]

$\quad\quad$ M: thickness of riverbed [L]

Evapotranspiration

The Evapotranspiration (ET) Package simulates the effects of plant transpiration and direct evaporation in moving water from the saturated groundwater regime. MODFLOW provides two possibilities to locate the evapotranspiration cells:

1. The evapotranspiration is applied only to cells in the top grid layer.

2. The evapotranspiration cell for each vertical column is specified by the user in the layer indicator array. It indicates the layer from which ET is removed.

After selecting the menu item "Evapotranspiration", you can select an option from a dialog box and then specify the following data by using the grid editor:

- maximum ET rate (volume of water per unit area per time unit [L/T])

- elevation of ET surface [L]

- ET extinction depth [L]

- layer indicator array [-] (required only if option 2 is chosen, note that the value of the layer indicator array must not be zero)

General-head boundary

The process of specifying data into the General-head boundary (GHB) Package is similar to that of the Drain Package. Two data types are required for each GHB-cell:

- hydraulic conductance [L^2/T] of the interface between the aquifer cell and the boundary
- head on the boundary

Recharge

The Recharge (RCH) package is designed to simulate areally-distributed recharge to the groundwater system. In MODFLOW, there are three ways to apply groundwater recharge to the model:

1. Recharge is only applied to the top grid layer.
2. Vertical distribution of recharge is specified in the layer indicator array. The layer indicator array defines the layer in each vertical column where recharge is applied.
3. Recharge is applied to the highest active cell in each vertical column. A constant-head cell intercepts recharge and prevents deeper infiltration.

After selecting the menu item "Recharge", you can select an option from a dialog box and then specify the following data by using the grid editor:

- recharge flux [L/T].
- layer indicator array [-] (required only if option 2 is chosen, note that the value of the layer indicator array must not be zero)

Stream-aquifer relation

To simulate stream-aquifer relation, MODFLOW needs the following information:

- sequential number of stream segment
- sequential number of stream reach of each segment
- streambed hydraulic conductance
- streamflow
- stream stage
- elevation of the bottom of the streambed
- elevation of the top of the streambed
- width of the stream channel
- slope of the stream channel in each reach
- Manning's roughness coefficient in each reach

The last three items are used only when the stream stage in each reach is calculated. After selecting the menu item "Stream-aquifer relation", the user will be asked to choose options and input control data in a dialog box. The grid editor helps the user to specify the data listed above. It uses the segment number of each cell to denote a stream. The user should specify the segment

number of each cell in the grid editor. Any cell which has a non-zero segment number, e.g. segment number 2, is a reach-cell of segment 2. The numbering scheme of figure 1b shown in page 4 of the documentation for the stream package from USGS (Prudic, 1989) will be used here. You may load the sample data (EXAMPLE.*) provided in the distribution diskettes and choose the stream package in the "Packages" menu to review the example concerning the numbering of segments and reaches.

4.2.5 The "Solver" menu

To calculate the hydraulic heads, a system of linear equations must be solved. In MODFLOW, the following iterative methods are available:

SIP: Strongly Implicit Procedure (Stone, 1968)

SSOR: Slice-Successive Overrelaxation

PCG2: Preconditioned Conjugate Gradient 2 (Hill, 1990a)

These solution methods can be selected from the "Solver" menu (Fig. 4.27). The selected method is indicated by a symbol » in the front of the corresponding menu item.

Fig. 4.27: The "Solver" menu

The detailed explanation of these solution methods is given in the MODFLOW documentation and Hill (1990a). In most cases, the choice of a solver depends on the problem itself. It is difficult to determine which solution method is the most efficient for solving all problems. Various comparisons between the solution methods have therefore been performed by many researchers.

Some can be found in Trescott (1977), Kuiper (1981), Behie et al. (1983), Scandrett (1989), and Hill (1990b).

The menu items of the "Solver" menu are described follows:

About Solvers:
Shows general information about the available solvers

SIP:
After selecting this menu item, a dialog box will come up and ask for parameters for solving the system of linear equations (Fig. 4.28). In addition to the parameters shown on Fig. 4.28, SIP requires the input of the parameters IPCALC, WSEED and IPRSIP. PREMOD uses the default values 1, 0, and 1 for these parameters, respectively. In most cases, you will not need to change these default values. For detailed descriptions of these parameters, please refer to the input instructions of the SIP Package.
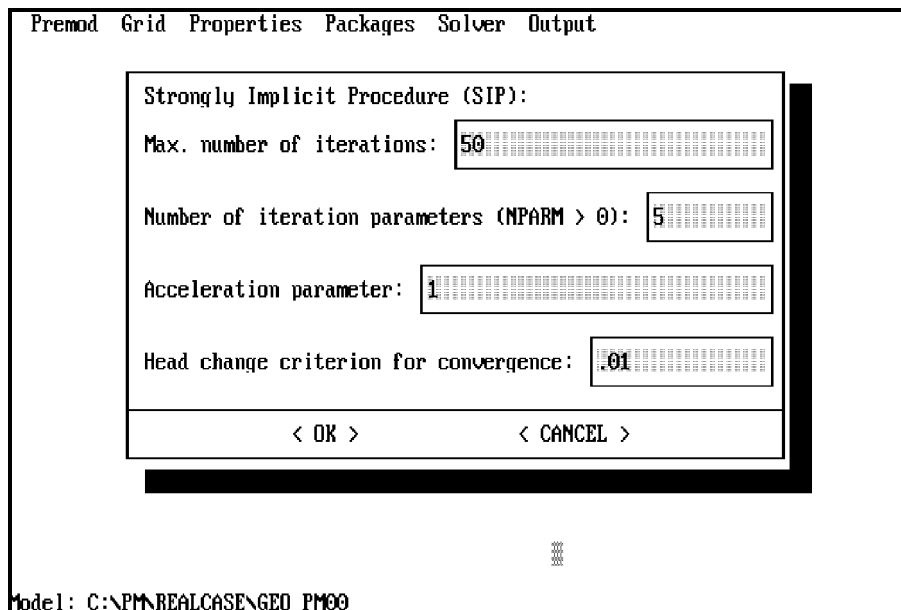
Fig. 4.28: Parameters for SIP

SSOR:
After selecting this menu item, a dialog box will come up, and ask for parameters for the SSOR Package (Fig. 4.29).
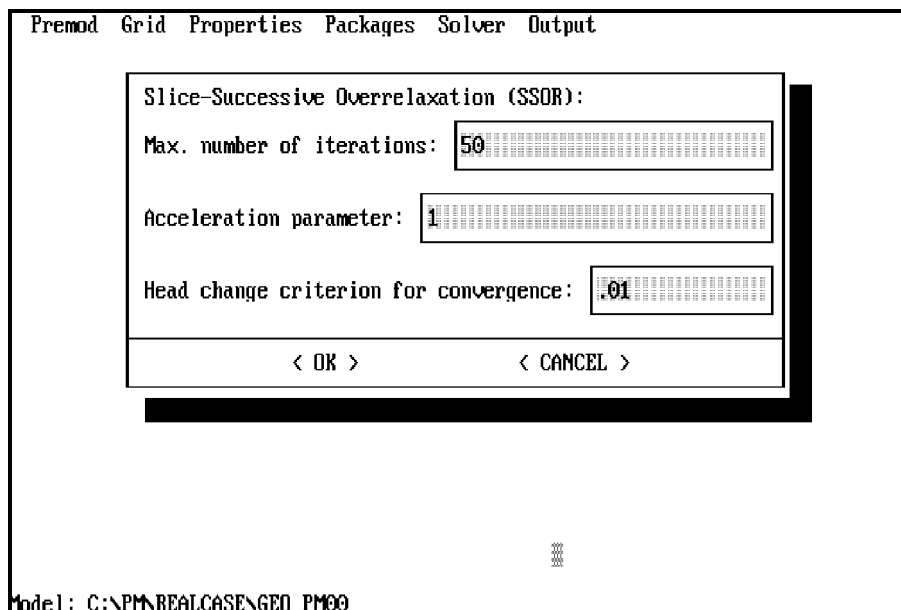
Fig. 4.29: Parameters for SSOR

PCG2:

After selecting this menu item, a dialog box will come up, and ask for parameters for the PCG2 Package (Fig. 4.30). The options are described as follows:

● Preconditioning method:

The PCG2 Package provides two preconditioning methods:

- MICCG: Modified Imcomplete Cholesky preconditioner (Axelsson and Lindskog, 1986)

- POLCG: least-squares polynomial preconditioner (Saad, 1985).

MICCG is developed for use on scalar computers and POLCG is developed for use on vector computers or to conserve computer storage. Hill (1990a, 1990b) points out that POLCG is not as efficient as SIP or MICCG on scalar computers and indicates that for three-dimensional, non-linear problems, SIP is generally a good alternative to consider.

● Printing from the solver:

If the first option is chosen, the extreme head changes and residuals will be printed in the simulation report file of MODFLOW. Otherwise, the printing will be suppressed.

● Printout interval for PCG:

The extreme head changes and residuals are printed for each iteration of a time step whenever the time step is an even multiple of the printout interval. The printout also occurs at the end of each stress period regardless of the user-specified printout interval.

● Maximum number of outer iterations:

For a linear problem, this number should be 1, unless more than 50 inner iterations are required. A larger number is required for a nonlinear problem.

● Maximum number of inner iterations:

A value of 30 will be sufficient for most linear problems. For nonlinear problems, this number usually ranges from 3 to 10.

● Head change criterion for convergence (in units of length [L]):

When the maximum absolute value of the head change at all cells during an iteration is less than or equal to this criterion and the residual criterion is satisfied (see below), iteration stops. The default value of this criterion is 0.01.

● Residual criterion for convergence (in units of cubic length per time [L^3/T]):

When the maximum absolute value of the residual at all cells during an iteration is less than or equal to this criterion and the head change criterion is satisfied (see above), iteration stops. The default value of this criterion is 0.01.

● Relaxation parameter:

This parameter is required only if MICCG is used. Usually, this parameter equals 1.00 but for some problems a value of 0.99, 0.98 or 0.97 will reduce the number of iterations required for convergence. The default value of this parameter is 1.00.

● Calculate the upper bound of the maximum eigenvalue:

If you are using the least-squares polynomial preconditioner (POLCG), you have to decide whether the upper bound on the maximum eigenvalue of the coefficient matrix A should be estimated or not (Fig. 4.31). In POLCG, the upper bound is estimated as the largest sum of the absolute values of the components in any row of the coefficient matrix A. The upper bound is used for calculating coefficients to optimize convergence. For a scaled matrix in POLCG, the upper bound is generally close to 2.

If you choose "NO" for this option, a value of 2 will be used for the upper bound.

```
 Premod  Grid  Properties  Packages  Solver  Output

    Preconditioning method:    [X] Modified Imcomplete Cholesky
                               [ ] Polynomial

    Printing from the solver: [ ] Printout all available information
                              [X] Printout the number of iterations only
                              [ ] Suppress all printing




    Printout interval for PCG:                  1
    Maximum number of outer iterations:         100
    Maximum number of inner iterations:         15
    Head change criterion for convergence:      .001
    Residual criterion for convergence:         .001
    Relaxation parameter:                       1

    < OK >    < CANCEL >

Model: C:\PM\REALCASE\GEO PM00
```

Fig. 4.30: Parameters for PCG2. MICCG is chosen

```
 Premod  Grid  Properties  Packages  Solver  Output

    Preconditioning method:    [ ] Modified Imcomplete Cholesky
                               [X] Polynomial

    Printing from the solver: [ ] Printout all available information
                              [X] Printout the number of iterations only
                              [ ] Suppress all printing

    Calculate the upper bound on
    the maximum eigenvalue:   [X] YES    [ ] NO

    Printout interval for PCG:                 1
    Maximum number of outer iterations:        100
    Maximum number of inner iterations:        15
    Head change criterion for convergence:     .001
    Residual criterion for convergence:        .001


    < OK >    < CANCEL >

Model: C:\PM\REALCASE\GEO PM00
```

Fig. 4.31: Parameters for PCG2. Polynomial is chosen.

4.2.6 The "Output" menu

This menu is used to control the frequency and amount of simulation results of MODFLOW that will be printed or saved. The primary result of a MODFLOW simulation is head distribution. In addition, drawdowns, volumetric water budget and cell-by-cell flow terms can be calculated by MODFLOW. The user can turn on or off one output item by selecting the corresponding menu item from the "Output" menu (Fig. 4.32). The symbol » in front of the menu item shows whether an item is turned on or not.

There are two ways to save these results. One is to save them in the simulation report file, the other is to save them separately in several binary files. By default, head distribution, drawdowns and the cell-by-cell flow terms will be saved separately. This is indicated by the symbol » in the front of the menu item "Output to several files". In **PM**, the default filenames of these results are HEADS.DAT, DDOWN.DAT, and BUDGET.DAT, respectively. The volumetric budget is always given in the simulation report file of MODFLOW. In **PM**, the default filename of the report file is OUTPUT.DAT.

The user may choose the option of saving all results in the simulation report file by selecting the menu item "Output to a single file". However, **if the user plans to run MODPATH and the postprocessors provided by PM, the results must be saved separately in binary files.**

The output frequency can be specified by selecting the menu item "Output frequency" from the "Output" menu. The output is produced for each n-th stress period and each m-th time step where n is the output frequency for the stress periods and m is output frequency for the time steps (Fig. 4.33). Note that results for the first and last stress periods and time steps are always saved. If the output frequency is not specified, both n and m will be set to 1, meaning that the output will be produced for each stress period and each time step. When choosing the output frequency, one should be aware of the fact that for a transient simulation, the head, drawdown and budget files can become very large. The Output frequency should therefore be chosen carefully unless you are doing the model calculation on a computer with large storage capacity.
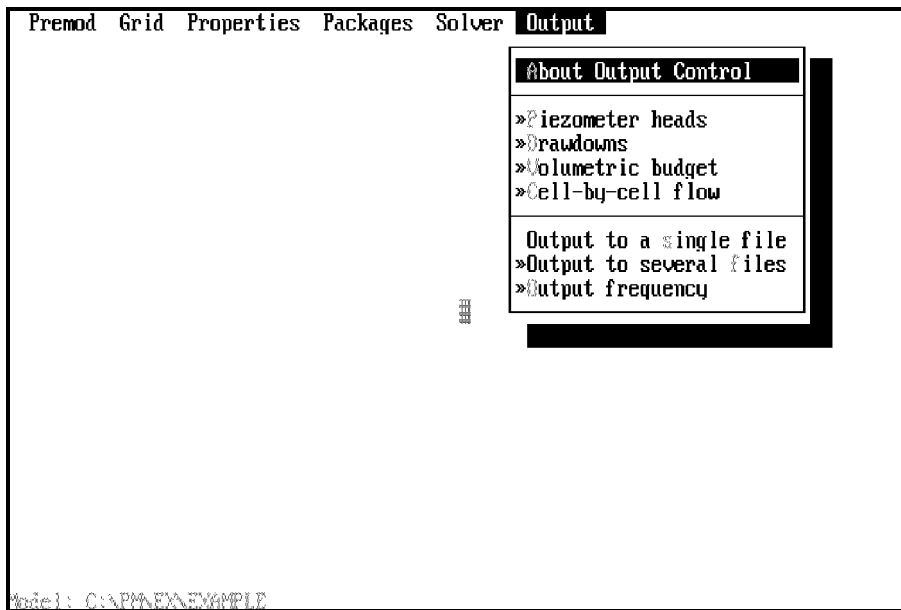
Fig. 4.32: The "Output" menu
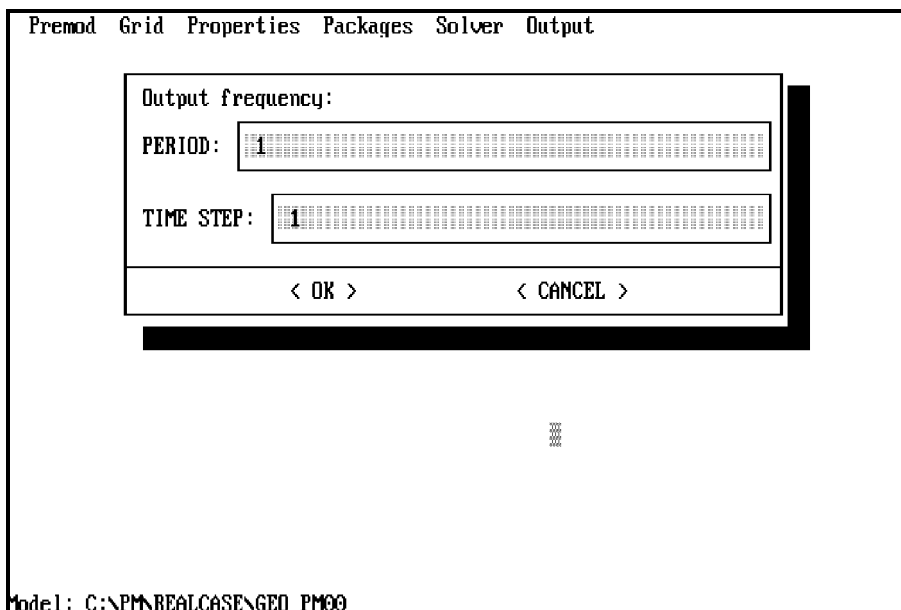
Fig. 4.33: Specification of the output frequency

4.3 PREMT3D - Preprocessor for MT3D

After the flow model is constructed and calibrated, you can use the preprocessor PREMT3D to prepare data for the transport model MT3D (Zheng, 1990). The MT3D transport model uses a mixed Eulerian-Lagrangian approach to the solution of the three-dimensional advective-dispersive-reactive equation and is based on the assumption that changes in the concentration field will not affect the flow field measurably. This allows the user to construct and calibrate a flow model independently. The calculated hydraulic heads and flow terms will be retrieved by MT3D.

The preprocessor PREMT3D retrieves the model information from the binary data files created by the preprocessor PREMOD. This includes not only the model dimension and the hydraulic parameters but also sinks/sources for each stress period, e.g., well, recharge, evapotranspiration, etc. The data specified or modified in PREMOD will be transferred to PREMT3D. PREMT3D is called by selecting the menu item "Edit transport model" from the "Model" menu of the PM-shell. Like PREMOD, PREMT3D uses also pull-down menus. The menu bar of PREMT3D contains four menu titles (Fig. 4.34). The "PreMT3D" menu allows the specification of time parameters for the transport simulation. Through the use of the "Concentration" menu, you can specify the initial concentration, the boundary indicator array for the concentration field and the location of observation points. The "Packages" menu allows you to specify the concentration of sinks/sources and parameters for the Advection, Dispersion, and Chemical Reaction Packages. Use of the "Output" menu allows you to decide which simulation results will be saved and printed and also when they should be saved or printed.

```
 PreMT3D  Concentration  Packages  Output









                                    ▓



















Model: C:\PM\REALCASE\GEO_PM00
```
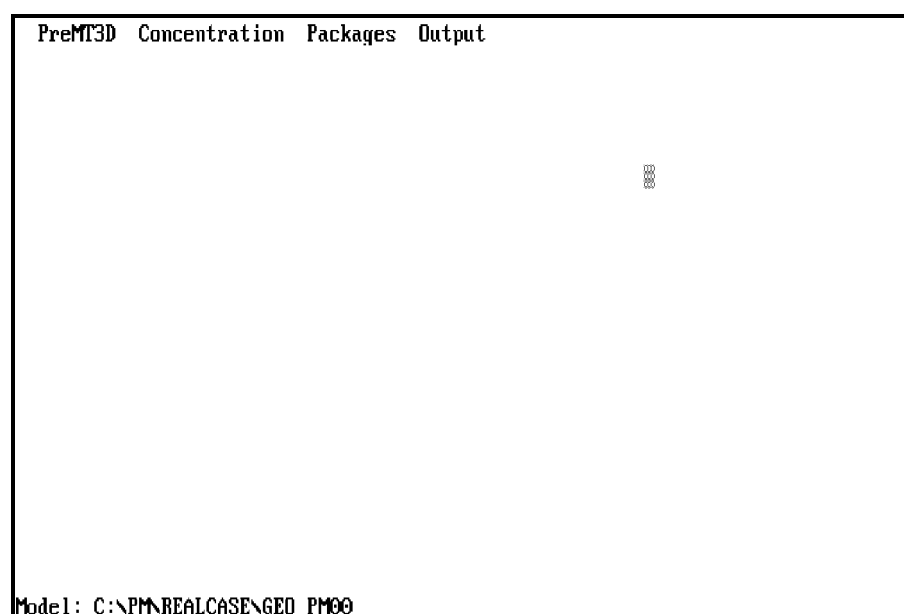
Fig. 4.34: Menu bar of PREMT3D

In the following sections, the use of each menu will be described in details.

4.3.1 The "PreMT3D" menu

The "PreMT3D" menu contains four menu items (Fig. 4.35), they are described as follows:
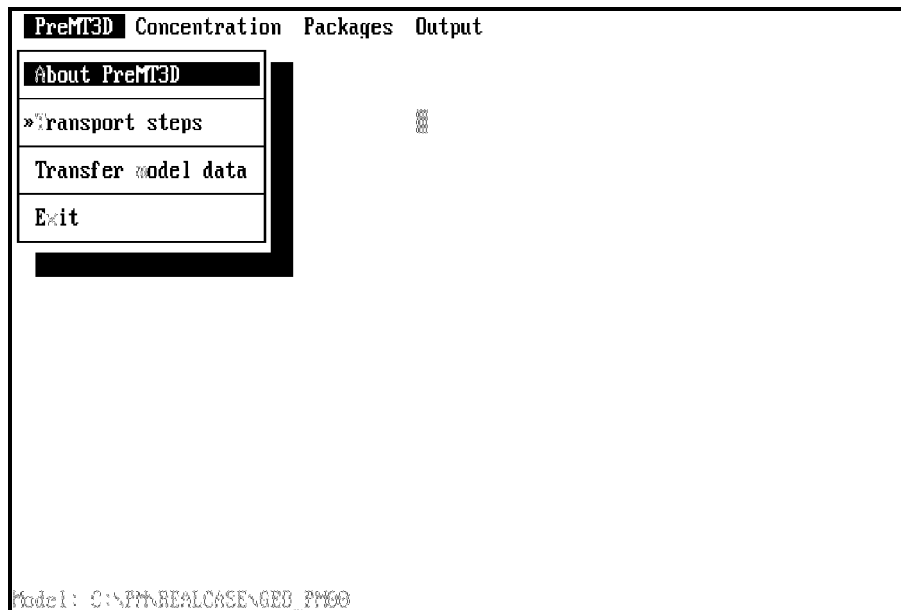
Fig. 4.35: The "PreMT3D" menu

Aboud PreMT3D:
Show general information about the Preprocessor PREMT3D.

Transport steps:
After selecting this menu item, a worksheet will come up and ask for time parameters for the transport simulation (Fig. 4.36). The use of the worksheet is described in section 4.2.1. The transport stepsize and the maximum number of transport steps allowed for one time step (of the flow simulation) are entered for each stress period. **The length of stress periods and the number of time steps must be specified in PREMOD, even if you have a steady-state flow model.**

Transfer model data:
To reduce the processing time, PREMT3D internally saves model data in binary files. Through a translator, these binary files will be converted into ASCII files which are actually used by MT3D. This translator is called by selecting the menu item "Transfer model data". If this menu item is colored in gray, the translator cannot be loaded and the computer will beep. This means that the model data is not complete.

> **Please note that "Transfer model data" must be performed whenever you have made changes in your model data. Otherwise, the ASCII model files will not be modified.**

Exit:

To exit PREMT3D and return to the PM-shell, select this menu item.

```
PreMT3D: Transport stepsize
┌─────────┬─────────┬─────────┬──────────────────────────┐
│    SP   │   DT0   │  MXSTRN │                          │
├─────────┼─────────┼─────────┼──────────────────────────┤
│     1   │      0  │   10000 │                          │
│     2   │      0  │   10000 │                          │
│     3   │      0  │   10000 │                          │
│     4   │      0  │   10000 │                          │
│     5   │      0  │   10000 │                          │
│     6   │      0  │   10000 │                          │
│     7   │      0  │   10000 │                          │
│     8   │      0  │   10000 │                          │
│     9   │      0  │   10000 │                          │
│    10   │      0  │   10000 │                          │
└─────────┴─────────┴─────────┴──────────────────────────┘
<ENTER>:EDIT  <ESC>:CANCEL  <Alt-Z>:SAVE/EXIT  <PgUp> <PgDn> ↑ ↓ ← →

SP is the stress period
DT0 is the user-specified transport stepsize. Setting DT0 to 0 causes the
   model-calculated DT0 to be used in the simulation.
MXSTRN is the maximum number of transport steps allowed for one time step
   (of the head solution)

Model: C:\PM\REALCASE\GEO_PM00
```

Fig. 4.36: Time parameters for transport simulations

4.3.2 The "Concentration" menu

The "Concentration" menu contains four menu items (Fig. 4.37). The symbol » shown in the front of a menu item indicates that the data has been specified. The following describes the menu items:

About concentration:

Provides a short description of the use of the "Concentration" menu.

ICBOUND (Boundary array):

ICBOUND is the boundary indicator array for the concentration field. This array can be specified by using the zones editor or the grid editor. IF ICBOUND=0, the cell is an inactive concentration cell. In MT3D, no-flow or dry cells are automatically converted to inactive cells. Furthermore, active head cells can be treated as inactive concentration cells to minimize the area needed for transport simulation, as long as the solute transport is insignificant near those cells.

IF ICBOUND<0, the cell is a constant concentration cell. The starting concentration is defined

by using the menu item "Starting concentration" and remains the same at the cell throughout the entire simulation. A constant head cell may or may not be a constant concentration cell.

IF ICBOUND>0, the cell is a variable (active) concentration cell.

Starting concentration:
The concentration at the beginning of the simulation can be specified by using the zones editor or the grid editor. The grid editor allows you to load the concentration field from a previous run into the grid. For details, see Appendices E and F.

Observation points:
The location of observation points can be specified by using the zones editor or the grid editor. A non-zero cell value indicates that the cell is an observation point. In PREMT3D, a maximum of 999 observation points are allowed.

Fig. 4.37: The "Concentration" menu

4.3.3 The "Packages" menu

The "Packages" menu of PREMT3D is divided in two parts. You may use the grid editor to specify the concentration of point- or areally-distributed sources or sinks by selecting a corresponding menu item from the first part of the "Packages" menu. Point sinks or sources include wells, drains, rivers (or streams), and general head-dependent boundary cells. Recharge and evapotranspiration are treated as areally distributed sinks and sources. To help the user locating the exact position of the point sinks or sources, the sinks/sources cells will be colored in

light blue.

If a type of sinks or sources is not used in the flow simulation, the corresponding menu item will be colored in gray and cannot be used. You may or may not specify the concentration for the sources or sinks when they are used in the flow simulation. If concentration of sources or sinks is not specified, the default value for the concentration is zero. If an activated sinks/sources or package is no longer necessary for a simulation, it can be switched off by selecting the corresponding menu item again.

The advection, dispersion and chemical reaction packages can be activated by selecting the corresponding menu item in the second part of the "Packages" menu. The symbol » indicates whether a package is activated or not. The user-specified data will not be lost by deactivating a menu item. That is, when you select the menu item again, the data will automatically be reloaded.

The following paragraph will describe the use of the menu items "Advection", "Dispersion" and "Chemical reaction".
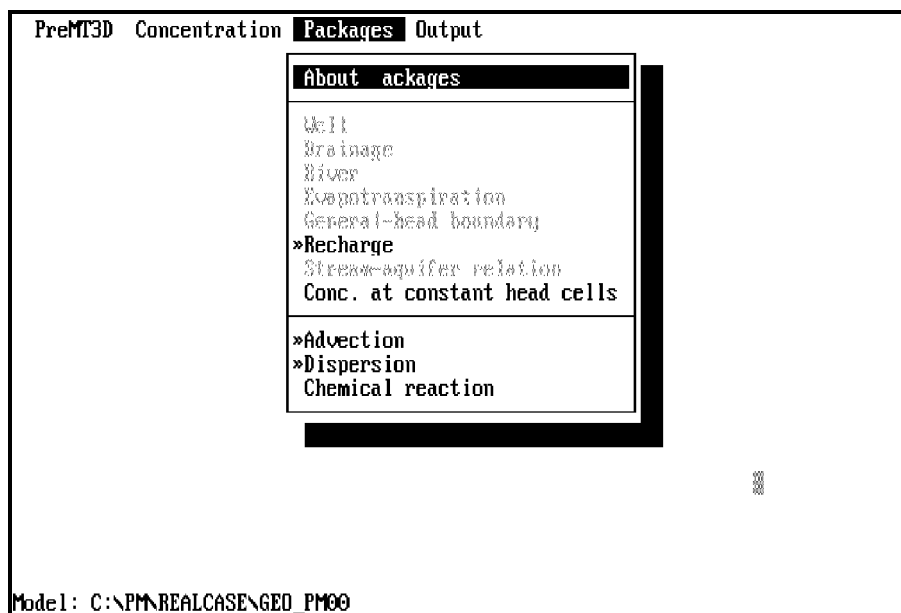
Fig. 4.38: The "Packages" menu of PREMT3D

Advection:

MT3D provides four methods for solving the advection term. They are the forward tracking method of characteristics (MOC), the backward-tracking modified method of characteristics (MMOC), the hybrid of MOC and MMOC (HMOC), and the upstream finite difference method. You can choose a method from the dialog box shown in Fig. 4.39. The Courant number and the maximum number of total moving particles (MXPART) should be chosen carefully. If MXPART

is exceeded during a transport simulation, the simulation will be terminated without displaying a message on the screen. If you have selected the MOC, MMOC or HMOC solution scheme, PREMT3D will prompt you to select a particle tracking algorithm and to specify parameters as shown in Fig. 4.40, 4.41 and 4.42, where DCCELL is the relative cell concentration gradient. Although most of the parameters in the dialog box are self-explanatory, you can find detailed explanations of each parameter and how the Advection Package works in the MT3D program documentation.

```
 PreMT3D  Concentration  Packages  Output

┌───────────────────── Advection ─────────────────────┐
│Advection solution scheme:                            ██
│Method Of Characteristics (MOC)......................[ ]│
▓│Modified Method Of Characteristics (MMOC)............[ ]│
│Hybrid MOC/MMOC (HMOC)...............................[X]│
│Upstream finite difference method....................[ ]│
│                                                      │
│                                                      │
│Courant number.........................(PERCEL)= .75  │
│Maximum number of total moving particles allowed.....(MXPART)= 600000│
│                                                      │
│                                                      │
│PERCEL is the Courant number, which is equivalent to the number of cells│
│through which a particle is allowed to move, in any direction for one│
│transport step. PERCEL is used to calculate the maximum allowed stepsize│
│for particle tracking. Generally, 0.5 <= PERCEL <= 1. If the upstream│
│finite difference method is used for solving the advective transport,│
│PERCEL must not exceed 1. MXPART is the maximum total number of particles│
│allowed, and is used only when MOC or HMOC are selected.│
│                                                      │
│                                                      │
│  < OK >       < CANCEL >                             │
└──────────────────────────────────────────────────────┘
     ████████████████████████████
Model: C:\PM\REALCASE\GEO PM00
```

Fig. 4.39: Selection of an advection soluton scheme

```
 PreMT3D  Concentration  Packages  Output

┌─────────────────── Advection (MOC) ───────────────────┐
│Particle tracking algorithm:                          ██
│First-order Euler algorithm..........................[ ]│
▓│Fourth-order Runge-Kutta algorithm...................[X]│
│Runge-Kutta algorithm is used in sinks/sources cells and the│
│cells next to sinks/sources, otherwise Euler algorithm is used.......[ ]│
│                                                      │
│Concentration weighting factor ..........................(WD)= .5  │
│Negligible relative concentration gradient...........(DCEPS)= .00001│
│Pattern for initial placement of particles...........(NPLANE)= 2│
│Number of particles per cell in case of DCCELL<=DCEPS...(NPL)= 0│
│Number of particles per cell in case of DCCELL> DCEPS...(NPH)= 20│
│Minimum number of particles allowed per cell..........(NPMIN)= 2│
│Maximum number of particles allowed per cell..........(NPMAX)= 30│
│Multiplier for the particle number at source cells...(SRMULT)= 1│
│                                                      │
│                                                      │
│  < OK >       < CANCEL >                             │
└──────────────────────────────────────────────────────┘
     ████████████████████████████
Model: C:\PM\REALCASE\GEO PM00
```

Fig. 4.40: Parameters required by MOC

```
PreMT3D  Concentration  Packages  Output

┌──────────────────── Advection(MMOC) ───────────────────┐
│Particle tracking algorithm:                            │
│First-order Euler algorithm......................[ ]    │
│Fourth-order Runge-Kutta algorithm...............[X]    │
│Runge-Kutta algorithm is used in sinks/sources cells and the │
│cells next to sinks/sources, otherwise Euler algorithm is used.......[ ] │
│                                                        │
│Concentration weighting factor ..........(WD)= .5       │
│Negligible relative concentration gradient...........(DCEPS)= .00001 │
│Pattern for placement of particles for sink cells....(NLSINK)= 2 │
│Number of particles used to approximate sink cells...(NPSINK)= 20 │
│                                                        │
│                                                        │
│                                                        │
│                                                        │
│                                                        │
│                                                        │
│   〈 OK 〉        〈 CANCEL 〉                          │
└────────────────────────────────────────────────────────┘

Model: C:\PM\REALCASE\GEO PM00
```

Fig. 4.41: Parameters required by MMOC

```
PreMT3D  Concentration  Packages  Output

┌──────────────────── Advection(HMOC) ───────────────────┐
│Particle tracking algorithm:                            │
│First-order Euler algorithm......................[ ]    │
│Fourth-order Runge-Kutta algorithm...............[X]    │
│Runge-Kutta algorithm is used in sinks/sources cells and the │
│cells next to sinks/sources, otherwise Euler algorithm is used.......[ ] │
│                                                        │
│Concentration weighting factor ..........(WD)= .5       │
│Negligible relative concentration gradient...........(DCEPS)= .00001 │
│Pattern for initial placement of particles...........(NPLANE)= 2 │
│Number of particles per cell in case of DCCELL<=DCEPS...(NPL)= 20 │
│Number of particles per cell in case of DCCELL> DCEPS...(NPH)= 20 │
│Minimum number of particles allowed per cell..........(NPMIN)= 2 │
│Maximum number of particles allowed per cell..........(NPMAX)= 30 │
│Multiplier for the particle number at source cells...(SRMULT)= 1 │
│Pattern for placement of particles for sink cells....(NLSINK)= 2 │
│Number of particles used to approximate sink cells...(NPSINK)= 20 │
│Criterion for controlling the selective use of either of │
│MOC or MMOC in the HMOC solution scheme .............(DCHMOC)= .0001 │
│   〈 OK 〉        〈 CANCEL 〉                          │
└────────────────────────────────────────────────────────┘

Model: C:\PM\REALCASE\GEO PM00
```

Fig. 4.42: Parameters required by HMOC

Dispersion:

After having selected this menu item, a worksheet will come up, and prompt you to enter the parameters TRPT, TRPV and DMCOEF for each layer (Fig. 4.43). The use of the worksheet is described in section 4.2.1. After having saved the parameters, you may use the zones editor or the grid editor to specify the longitudinal dispersivity (α_L, unit: [L]) for each cell in the grid.

```
PreMT3D: Dispersion Package

 LAYER |        TRPT |        TRPV |       DMCOEF |
       |             |             |              |
     1 |          .1 |          .1 |            0 |
     2 |          .1 |         .05 |            0 |
     3 |          .1 |         .05 |            0 |
       |             |             |              |
       |             |             |              |
       |             |             |              |
       |             |             |              |
       |             |             |              |

<ENTER>:EDIT   <ESC>:CANCEL   <Alt-Z>:SAVE/EXIT   <PgUp> <PgDn> ↑ ↓ ← →

TRPT is the ratio of the horizontal transverse dispersivity to the longitudinal
     dispersivity.
TRPV is the ration of the vertical transverse dispersivity to the longitudinal
     dispersivity.
DMCOEF is the effective molecular diffusion coefficient [L^2/T]


Model: C:\PM\REALCASE\GEO PM00
```

Fig. 4.43: Parameters for the Dispersion Package

Chemical reaction:

Chemical reactions supported by the MT3D transport model (version 1.8) include equilibrium-controlled sorption reactions and first-order irreversible rate reactions, such as radioactive decay or biodegradation. This is selected from an option box (Fig.4.44). If a type of sorption isotherm or a first-order rate reaction is simulated, PREMT3D will prompt you to enter the required parameters in a worksheet. Fig. 4.45 shows an example with parameters for the linear isotherm and the first-order rate reaction.

```
 PreMT3D  Concentration  Packages  Output
 ┌──────────────────── Chem. reaction ────────────────────┐
 │Type of sorption:                                        │
 │Linear isotherm.......................................[X]│
 │Freundlich isotherm...................................[ ]│
 │Langmuir isotherm ....................................[ ]│
 │No sorption...........................................[ ]│
 │                                                         │
 │Simulation of the radioactive decay or biodegradation  [ ] YES   [X] NO │
 │                                                         │
 │                                                         │
 │                                                         │
 │                                                         │
 │                                                         │
 │                                                         │
 │   < OK >        < CANCEL >                               │
 └─────────────────────────────────────────────────────────┘
Model: C:\PM\REALCASE\GEO PM00
```
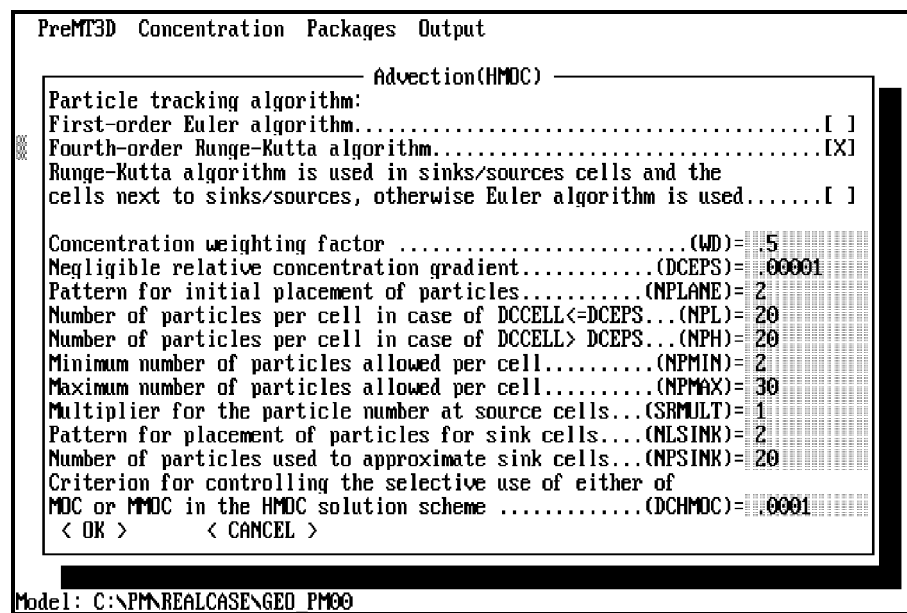
Fig. 4.44: Specification of the type of sorption

```
PreMT3D: Chemical Reaction Package
┌─────────┬───────────┬───────────┬──────────┬───────────┬───────────┐
│  LAYER  │      RHOB │       SP1 │      SP2 │       RC1 │       RC2 │
├─────────┼───────────┼───────────┼──────────┼───────────┼───────────┤
│       1 │      1700 │    .00012 │        0 │     1E-08 │     1E-08 │
│       2 │      1600 │    .00008 │        0 │     1E-08 │     1E-08 │
│       3 │      1600 │    .00008 │        0 │     1E-08 │     1E-08 │
│         │           │           │          │           │           │
│         │           │           │          │           │           │
│         │           │           │          │           │           │
│         │           │           │          │           │           │
│         │           │           │          │           │           │
│         │           │           │          │           │           │
└─────────┴───────────┴───────────┴──────────┴───────────┴───────────┘
<ENTER>:EDIT  <ESC>:CANCEL  <Alt-Z>:SAVE/EXIT  <PgUp> <PgDn> ↑ ↓ ← →

RHOB is the bulk density of the porous medium in the aquifer [M/L^3]
SP1 is the distribution coefficient (Kd) [L^3/M]
SP2 is not used
RC1 is the first-order rate constant for the dissolved phase [1/t]
RC2 is the first-order rate constant for the sorbed phase [1/t]

Model: C:\PM\REALCASE\GEO PM00
```

Fig. 4.45: Parameters for the Chemical Reaction Package

4.3.4 The "Output" menu

The transport model MT3D generates a standard simulation report file and several optional output files. The output of MT3D can be controlled by using the "Output" menu (Fig. 4.46). The simulation result terms, which are indicated by (ASCII) in Fig. 4.46, will be printed in the MT3D report file. In **PM**, the default filename of the report file is OUTPUT.MT3.

The calculated concentration field can also be saved in a default unformatted file 'MT3D.UCN' by activating the menu item 'Concentration (unformatted)'. This file can be used for a continuation run or for post-processing purposes. Selecting the menu item 'output frequency' enables you to specify the frequency of the output (Fig. 4.47). If the output frequency has not been specified, an output frequency of '0' will be used. This means that the results will only be saved or printed at the end of a stress period.

You can switch an output item on or off by selecting a corresponding menu item from the "Output" menu. The symbol » indicates whether an output item is chosen or not.
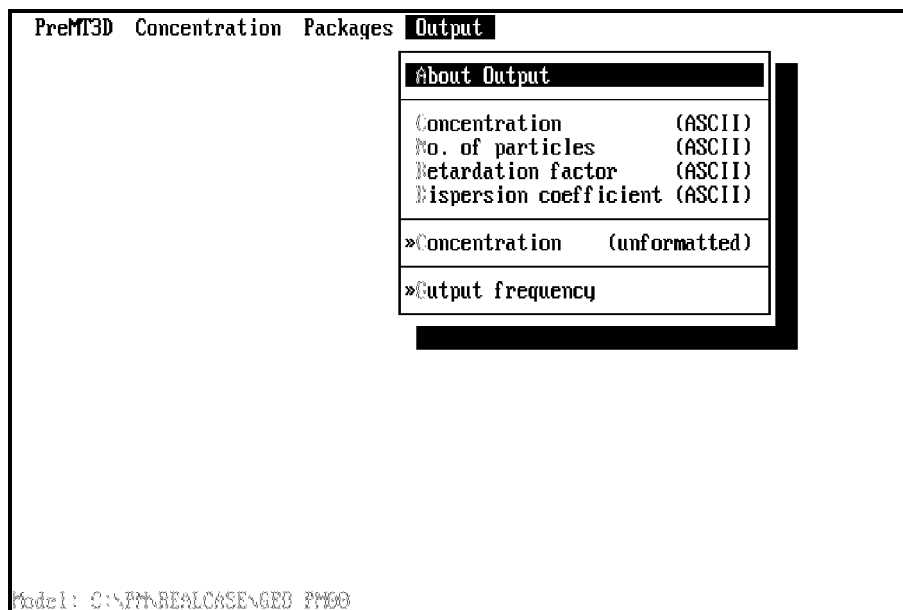
```
 PreMT3D  Concentration  Packages  ▐Output▌

                         ┌─────────────────────────────────┐
                         │▐About Output▌                    │
                         ├─────────────────────────────────┤
                         │ Concentration        (ASCII)     │
                         │ No. of particles     (ASCII)     │
                         │ Retardation factor   (ASCII)     │
                         │ Dispersion coefficient (ASCII)   │
                         ├─────────────────────────────────┤
                         │»Concentration     (unformatted)  │
                         ├─────────────────────────────────┤
                         │»Output frequency                 │
                         └─────────────────────────────────┘


 Model: C:\PM\REALCASE\GEO PM00
```

Fig. 4.46: The "Output" menu of PREMT3D

```
 PreMT3D  Concentration  Packages  Output

        ┌───────────────────────────────────────────────┐
        │ Output frequency:                              │
        │                                                │
        │   NPRS:  │-5░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░│  │
        │                                                │
        ├───────────────────────────────────────────────┤
        │          < OK >              < CANCEL >        │
        └───────────────────────────────────────────────┘


    ┌───────────────────────────────────────────────────────┐
    │ NPRS is a flag indicating the frequency of the output, │
    │ and also indicating whether the output frequency is    │
    │ specified in terms of total elapsed simulation time or │
    │ the transport step number.                             │
    │ if NPRS>0, simulation results will be printed or saved │
    │    at times as specified in the TIMPRS(NPRS) to be     │
    │    entered in the next table.                          │
    │ if NPRS=0, simulation results will not be printed or   │
    │    saved except at the end of each stree period        │
    │ if NPRS<0, simulation results will be printed or saved │
    │    whenever the transport steps is an even multiple of │
    │    NPRS                                                │
    └───────────────────────────────────────────────────────┘

 Model: C:\PM\REALCASE\GEO PM00
```
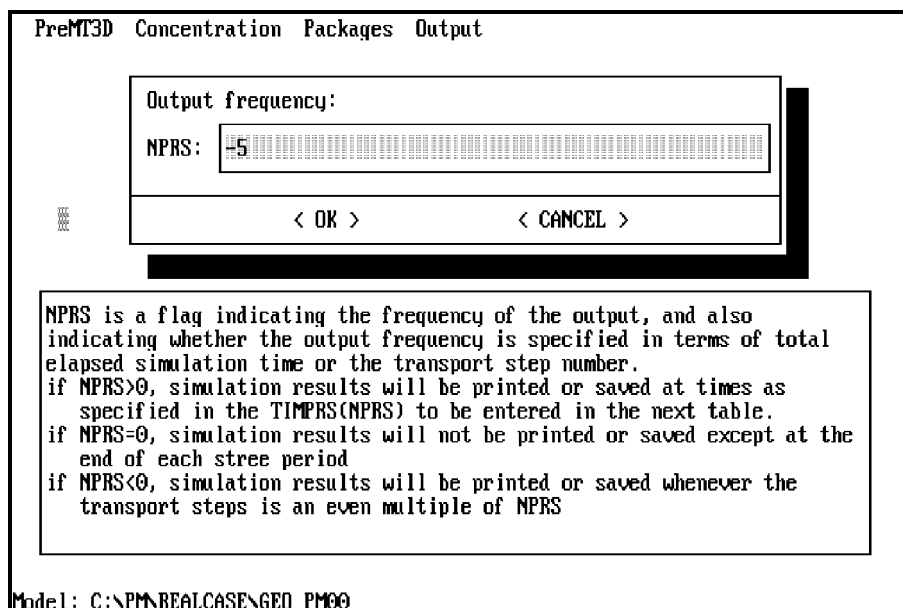
Fig. 4.47: Specification of the output frequency

5. Simulation of Groundwater Flow and Solute Transport

5.1 Simulation of groundwater flow with MODFLOW

As described in chapter 4, the preprocessor PREMOD internally saves the model data in binary files. A translator will retrieve these files and create ASCII model files for each package of MODFLOW. If MODFLOW is installed in the PM-directory, it can be called by selecting the menu item "MODFLOW-simulation" from the "Computation" menu of the PM-shell. The PM-shell uses the filenames listed in Tab. 2.1 to call MODFLOW.

During a simulation, MODFLOW uses the files given in Tab. 5.1 for saving the results. The result files are saved in the data-directory. After the simulation run, the PM-shell will call the program **PMCNV** to convert the binary head and drawdown files into ASCII. The converted ASCII files are 'HEADS.ASC' and 'DDOWN.ASC'. These ASCII files and the binary file 'BUDGET.DAT' will be used by the postprocessors provided by **PM**. In addition to these ASCII files, PMCNV will also save the head distribution in each layer at the last time step by using the filename Hxx, where xx is the layer number. The Hxx files are saved in the data-directory and can be read by the grid editor. This allows you to use the calculated heads for further simulations. For more information about "Continuation of a previous run", see Appendix F.

Simulation result	output file
head distribution	HEADS.DAT
drawdowns	DDOWN.DAT
cell-by-cell flow terms	BUDGET.DAT
simulation report file	OUTPUT.DAT

Tab. 5.1: The simulation results of MODFLOW

The following sections describe how to perform a groundwater simulation with various versions of MODFLOW supported by **PM**.

5.1.1 Running PM with the SSG-MODFLOW

After starting MODFLOW the following lines appear:

> The File-Name input unit is 99
> Enter the name of the File-Name input File:

Answer by typing **FLOWFILE.** The file-name input file 'FLOWFILE' contains the UNIT assignments, path and names of the input and output files. The names of the input files for each package are given in Appendix B.

'FLOWFILE' is created or modified whenever the translator is performed by selecting the menu item "Transfer model data" from the "Premod" menu (see section 4.2.1).

5.1.2 Running PM with the IGWMC-MODFLOW

After starting MODFLOW, the name and the full path of the model data for each selected package has to be typed at the prompt. The names of the input files for each package are given in Appendix B. The following shows an example. The model data are saved in the data-directory C:\PM\DATA and the Well and PCG2 Packages are used. The following underlined text should be typed at the prompt:

> Enter the file name for the ASCII output file,unit 6:
> C:\PM\DATA\OUTPUT.DAT
> Enter the file name for the BASIC Package file,unit 1:
> C:\PM\DATA\BAS.DAT
> Enter the file name for the BCF Package file,unit 11:
> C:\PM\DATA\BCF.DAT
> Enter the file name for the WELL Package file,unit 12:
> C:\PM\DATA\WEL.DAT
> Enter the file name for the PCG2 Package file,unit 20:
> C:\PM\DATA\PCG2.DAT
> Enter the file name for the OC Package file,unit 22:
> C:\PM\DATA\OC.DAT
> Enter the file name for binary head output, unit 51:
> C:\PM\DATA\HEADS.DAT

Enter the file name for binary drawdown output,unit 52:
C:\PM\DATA\DDOWN.DAT
Enter the file name for BCF cell-by-cell flux terms, unit 50:
C:\PM\DATA\BUDGET.DAT
Enter the file name for WELL cell-by-cell flux terms, unit 50:
C:\PM\DATA\BUDGET.DAT

> The filename for all flux terms must always be BUDGET.DAT and that for head and draw-down output HEADS.DAT and DDOWN.DAT, respectively. The postprocessors provided by PM will read these files from the data-directory.

5.1.3 Running PM with the SSPA-MODFLOW

The PM-shell calls the SSPA-MODFLOW by using the command

   MODF < MODFFILE

MODFFILE is a response file that contains the names of input and output files in the order required by the SSPA-MODFLOW. The names of the input files for each package of MOD-FLOW are given in Appendix B. The simulation results will be saved in the output files listed in Tab. 5.1.

'MODFFILE' is created or modified whenever the translator is performed by selecting the menu item "Transfer model data" from the "Premod" menu (see section 4.2.1).

5.1.4 Running PM with the user's MODFLOW:

The PM-shell calls the user's version of MODFLOW by using the filename 'MODFLOW.EXE'. The name of the input files for each package of MODFLOW are given in Appendix B. The input files are saved in the data-directory. If you intend to use the postprocessors of **PM**, you must use the filenames listed in Tab. 5.1 to save the simulation results in the data-directory, where your model data are saved.

5.2 Calculation of pathlines with MODPATH

If MODPATH is installed in the PM-directory, it can be called by selecting the menu item "MODPATH-particle tracking" from the "Computation" menu of the PM-shell. The PM-shell uses the filenames listed in Tab. 2.1 to call MODPATH. After starting MODPATH the following lines appear:

```
--------------------------------------------
MODPATH -- Version x.x
--------------------------------------------
ENTER NAME OF FILE CONTAINING NAMES AND UNITS OF DATA FILES:
```

Answer by typing **PATHFILE.** The file 'PATHFILE' contains the UNIT assignments, path and names of the input data files. The names of the input files for MODFLOW and MODPATH are given in Appendix B. MODPATH provides three modes for storing output data:

```
MODE 0 = ENDPOINTS AND STARTING POINTS ONLY
MODE 1 = FLOW LINE COORDINATES
MODE 2 = TIME SERIES DATA FOR SCATTER PLOTS
```

By default, the output data files will be saved in the same directory as MODPATH. These files are ENDPOINT, PATHLINE, and TIMESERS for the output mode 0, 1 and 2, respectively. These files will always be overwritten whenever MODPATH is called. The files PATHLINE and TIMESERS can be retrieved by the PM-postprocessor PATHLINE for creating graphics plots.

5.3 Simulation of contaminant transport with MT3D

If MT3D is installed in the PM-directory, it can be called by selecting the menu item "MT3D-Transport of contaminants" from the "Computation" menu of the PM-shell. The PM-shell calls MT3D by using the command

  MT3D < MT3DFILE

'MT3DFILE' is a response file. This file contains the names of input and output files in the order required by MT3D. It is created or modified whenever the translator is performed by selecting the menu item "Transfer model data" from the "PreMT3D" menu (see section 4.3.1). The names of the input files for each package of MT3D are given in Appendix B.

By default, the simulation report will be saved in the file 'OUTPUT.MT3' and the calculated concentration field in a binary file 'MT3D.UCN'. In addition, MT3D will saves a model grid configuration file 'MT3D.CNF' for postprocessing purposes. The file 'OUTPUT.MT3' is saved in the data-directory. When running MT3D, the files 'MT3D.UCN' and 'MT3D.CNF' are saved in the same directory as MT3D by turning on the output of unformatted concentrations. The files "MT3D.UCN" and "MT3D.CNF" will be overwritten whenever MT3D is called.

After a simulation run, the PM-shell will call the program **SAVELAST** provided by MT3D to extract the concentration at the last step and save it in a separate binary file (by default: 'RE-RUN.UCN') as the starting concentration for a continuation run. This binary file, however, cannot be directly examined and read by the grid editor of PREMT3D. To solve this problem, the PM-shell will call the program **MT3DCNV** to convert the binary concentration data of each layer in seperate ASCII files. The converted concentration data of each layer will be saved in the data-directory by using the filename Cxx, where xx is the layer number. The Cxx files can be read by the grid editor. This allows you to use the calculated concentration for further simulations. For more information about "Continuation of a previous run", see Appendix F.

6. Postprocessors

PM provides five postprocessors: 1) ISOLINE for generating head and drawdown contours, 2) PMWBLN (water balance) for the calculation of sub-regional water budgets, 3) PATHLINE for creating plot data files from the results of MODPATH, 4) PMHT for generating heads-time development curves for a transient simulation and 5) PMGRAF for creating graphic plots of the user-specified areally distributed data. In addition to these postprocessors, MODPATH-PLOT is also supported by **PM**. If MODPATH-PLOT is installed in the PM-directory, it can be called from the PM-shell.

The postprocessors are called by selecting a corresponding menu item from the "Analysis" menu of the PM-shell. Each of the postprocessors will automatically load the model grid configuration from the model data files saved in the data-directory.

The following sections describe the use of each of the postprocessors.

6.1 Head and drawdown contours (ISOLINE)

The program ISOLINE uses the ASCII head and drawdown files "HEADS.ASC" and "DDOWN.ASC" for generating contours. ISOLINE has four pull-down menus (Fig. 6.1). The menu items of each pull-down menu are described follows:
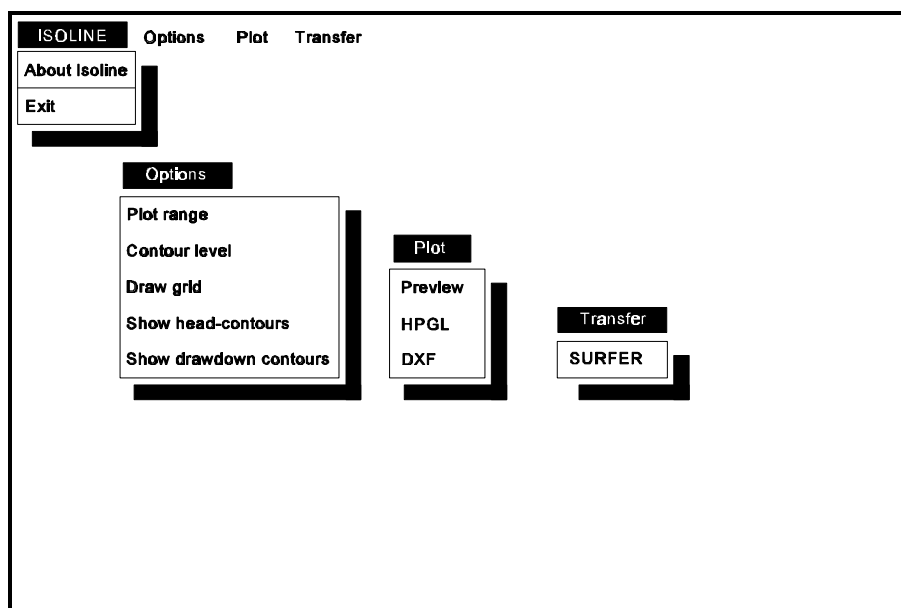
Fig. 6.1: The pull-down menus of ISOLINE

About Isoline:

Shows general information about ISOLINE

Exit:

Exits ISOLINE, and returns to the PM-shell

Plot range:

After selecting this menu item, a dialog box will come up and ask for the time parameters and the range for plotting contours (Fig. 6.2). The user can select the data at the desired step by specifying the number of stress period, time step and layer. The plot range within which the contours will be plotted is defined by the starting and ending column (X) and row (Y) indices. The coordinate system of the grid editor (see Fig. 4.4) will be used for specifying the indices.

```
 Isoline  Options  Plot  Transfer


                          ┌─── Plot range ───┐

        Number of layers = 3
        Number of stress periods = 1
        Number of time steps of stress period 1 = 1

        Stress period: 1      time step: 1      Layer: 1

        Range (Xmin,Ymin)-(Xmax,Ymax):
        Xmin:   1              Ymin: 1
        Xmax:  20              Ymax: 20


              < OK >              < CANCEL >


Model: C:\PM\EX\EXAMPLE
```
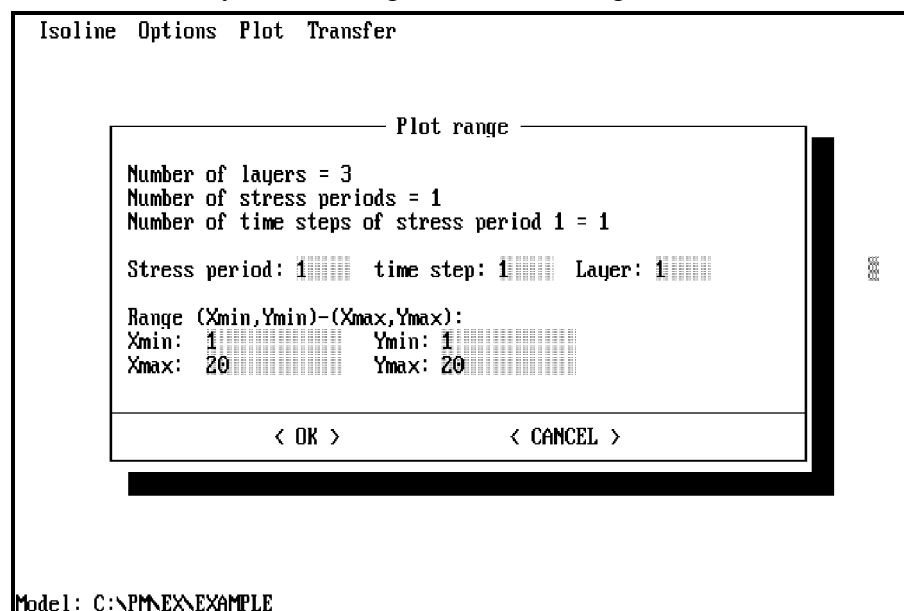
Fig. 6.2: Specification of the range for plotting contours

Contour levels:

By default, contour levels are automatically chosen such that 11 contours from the lower limit to the upper limit of the data will be plotted. The user can change the contour levels by specifying the increment, the upper and the lower limits of the contours in a dialog box.

Draw grid:

By default, the "Draw grid" option is not selected. If this option is selected, the model grid will be overlaid on the contour map. The "Draw grid" option can be switched off by selecting the menu item again. Whether the option is selected or not is indicated by the symbol » in the front of the menu item.

Show head-contours:

If this menu item is selected, ISOLINE will use the ASCII head file "HEADS.ASC" for plotting contours.

Show drawdown contours:

If this menu item is selected, ISOLINE will use the ASCII drawdown file "DDOWN.ASC" for plotting contours.

Preview:

Shows the contours on the screen.

HPGL:

Saves the contour plot in HPGL format. After selecting this menu item, a dialog box will come up and ask for the filename and the scale of the plot (Fig. 6.3). The default scale is set such that the plot fits on an A4 (297mm × 210mm) sheet.

```
Create HPGL-Metafile

SAVE HPGL-PLOT AS :   C:\PM\EX\EXAMPLE.PGL

Scale for drawing ....................[1 :]   5586

         < OK >              < CANCEL >
```
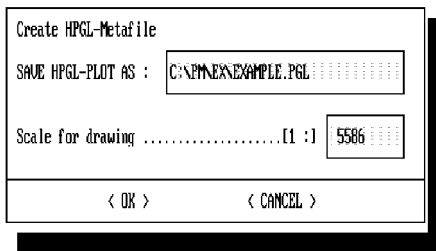
Fig. 6.3: Saving the contour plot in HPGL-format

DXF:

Saves the contour plot in DXF-format. After selecting this menu item, a dialog box will come up and ask for the filename. The plot can be output to match the model grid of the general map created by using PMCAD. This is done by selecting the option "match the map" in the dialog box (Fig. 6.4).
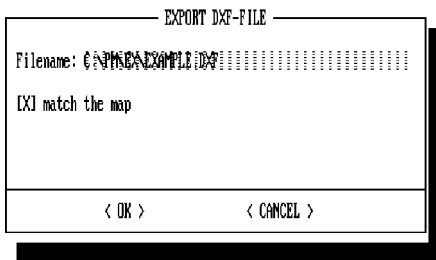
```
──────── EXPORT DXF-FILE ────────

Filename: C:\PM\EX\EXAMPLE.DXF

[X] match the map


         < OK >              < CANCEL >
```

Fig. 6.4: Save the contour plot in DXF format

SURFER:

Saves the grid data in the ".DAT" format, according to the convention used by the graphic package SURFER. In the ".DAT" format, the heads or drawdowns at each cell and the coordinate of each cell are saved.

6.2 Water balance (PMWBLN)

PM uses two programs to calculate water balance: 1) PMWBLN uses the grid editor for defining the zones for which the water balance should be calculated and 2) PMWBLF retrieves the locations of the zones and uses the cell-by-cell flow terms saved in the binary file 'BUDGET.DAT' to calculate the water budget for each sub-region and the entire model domain. After selecting the menu item "Water balance" from the "Analysis" menu of the PM-shell, PMWBLN will first be loaded. PMWBLN has 3 pull-down menus (Fig. 6.5). Each of the menu items is described follows:
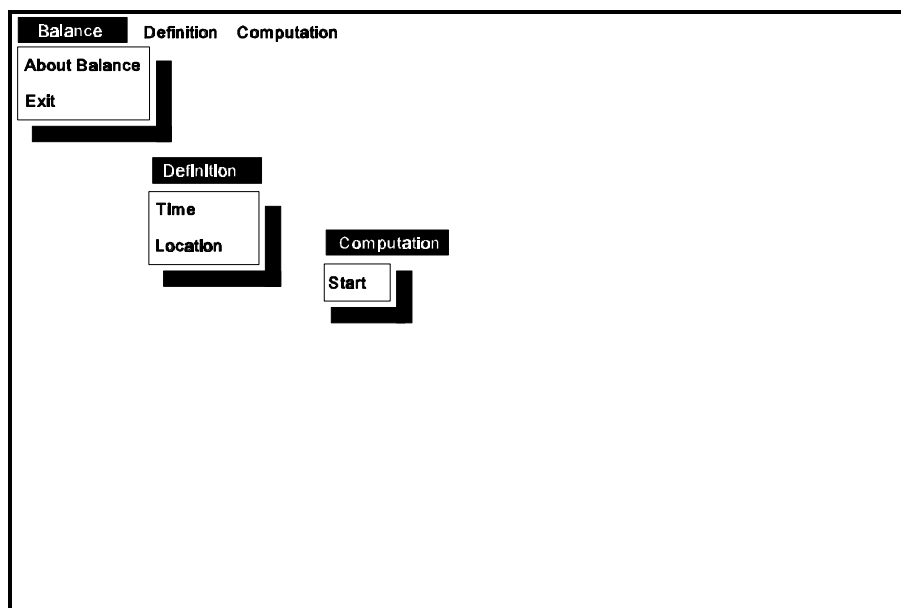

Fig. 6.5: The pull-down menus of PMWBLN

About balance:
Shows information about the program PMWBLN

Exit:
Exits PMWBLN, and returns to the PM-shell.

Time:

This menu item is used to specify the stress period and time step for which the water balance should be calculated.

Location:

After selecting this menu item, the grid editor will come up. The user can use the grid editor to define the sub-regions by specifying the region number to the model cells. For instance, the cells that have a value of 1 are cells of the sub-region 1. The maximum allowed number of sub-regions is 50.

Start:

After having specified the location and time, the program PMWBLF can be called by selecting this menu item for calculating of the water balance. The water balance is calculated for both the sub-regions in each layer and the entire model domain. The calculated water balance will be displayed on the screen and can be saved in a file or scrolled by using the functions displayed on the bottom of the screen (Fig. 6.6). The water balance is given for each zone in each layer.

```
 Balance  Definition  Computation


WATER BALANCE
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  1.0019344E-02 -1.0019344E-02
   HORIZ. EXCHANGE   4.6171751E-03  3.9885452E-04  4.2183204E-03
  EXCHANGE (UPPER)   0.0000000E+00  0.0000000E+00  0.0000000E+00
  EXCHANGE (LOWER)   5.6524668E-03  5.3623198E-06  5.6471047E-03
             WELLS   0.0000000E+00  0.0000000E+00  0.0000000E+00
            DRAINS   0.0000000E+00  0.0000000E+00  0.0000000E+00
          RECHARGE   1.3249996E-04  0.0000000E+00  1.3249996E-04
                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
  SUM OF THE LAYER   1.0402142E-02  1.0423562E-02 -2.1419488E-05

<Home> <PGUP> <PGDN> ↑ ↓ <ESC>:EXIT  <F1>:SAVE
Model: C:\PM\EX\EXAMPLE
```
Fig. 6.6: Water balance

Flows are considered 'IN' if they are entering a sub-region. The unit for the flows is [L^3/T]. The flow term "HORIZ. EXCHANGE" is the sum of fluxes which cross the boundary of a sub-region within a layer. The flow term "EXCHANGE (UPPER)" or "EXCHANGE (LOWER)" is the sum of fluxes which come from the upper or lower neighboring layer into a sub-region.

The balance for the entire model domain is attached at the end of the balance report. If you

compare the in- and outflows of "CONSTANT HEAD" with the volumetric budget of the entire model saved in the report file "OUTPUT.DAT", you may notice that they are different. In MODFLOW, the in- and outflows through each face of a constant head cell are calculated separately. The sum of all inflows and the sum of all outflows are given in the volumetric budget of the report file. However, only the sum of the in- and outflows to each constant head cell is saved in the file "BUDGET.DAT" which is used to calculate the 'IN' and 'OUT' terms of "CONSTANT HEAD". These terms are therefore different from the volumetric budget given in OUTPUT.DAT, although the total balance remains unchanged.

6.3 Pathlines (PATHLINE)

The program PATHLINE generates two plot types by using the result files 'PATHLINE' or 'TIMESERS' of the output mode 1 or 2 of MODPATH (see section 5.2). If both result files are not found in the PM-directory, PATHLINE will prompt you to run MODPATH. PATHLINE has three pull-down menus (Fig. 6.7). The following paragraphs describe the use of each menu item.
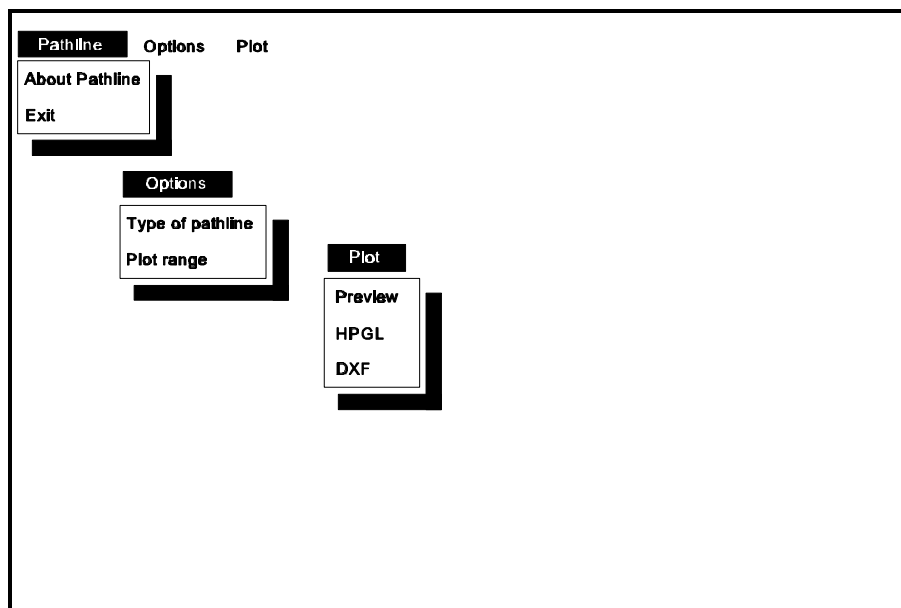

Fig. 6.7: The pull-down menus of PATHLINE

About pathline:
Shows the general information about PATHLINE

Exit:

Exits PATHLINE, and returns to the PM-shell.

Type of pathline:

PATHLINE generates two plot types by using the result files 'PATHLINE' or 'TIMESERS'. This can be selected from an option box (Fig. 6.8). If one of the result files is not saved in the PM-directory, the corresponding option vanishes.
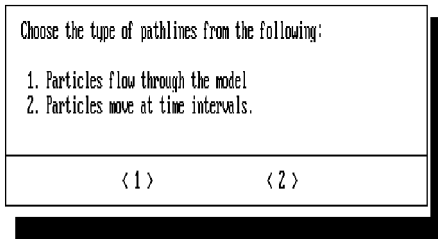
```
Choose the type of pathlines from the following:

1. Particles flow through the model
2. Particles move at time intervals.

              <1>          <2>
```

Fig. 6.8: Type of pathline

Plot range:

The plot range within which the pathlines will be plotted is defined by the starting and ending x-, y- and z-coordinates in two dialog boxes (Fig. 6.9 and Fig. 6.10). The origin of the coordinate system is located in the upper-left corner of the model grid. The positive x and y coordinates are in the directions of increasing column and row indices.
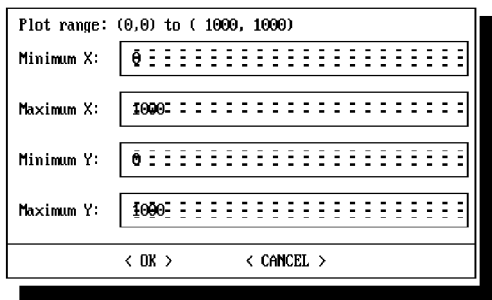
```
Plot range: (0,0) to ( 1000, 1000)
Minimum X:   0
Maximum X:   1000
Minimum Y:   0
Maximum Y:   1000
           < OK >      < CANCEL >
```

Fig. 6.9: Specification of the plot range in the x- and y-directions

```
Enter the lower and upper limits:
Minimum Z:   0
Maximum Z:   25
Scale factor for the height:  1
           < OK >      < CANCEL >
```
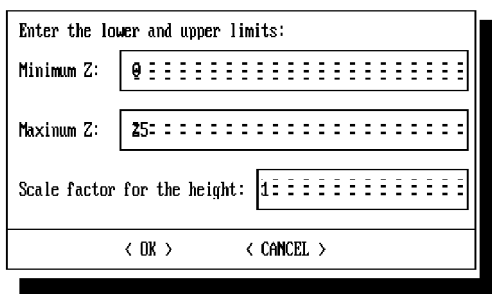
Fig. 6.10: Specification of the upper and lower limit of the plot range

Preview:

Shows the pathlines on the screen. Optionally, the projections of pathlines on the coordinate planes or a 3D-view of pathlines can be chosen from an option box (Fig. 6.11). If the first option is chosen, the projections of pathlines on the XY-, XZ- and YZ-planes will be shown on the screen (Fig. 6.12). If the 3D-view is chosen, PATHLINE will first show the top view of the model frame. It can be rotated about the x- and y-axis by using the arrow keys (Fig. 6.13). Once the view angle is decided, press the ENTER key to start the particles. If it is desired, you can press the ESC key to stop the particles and the ENTER key to start them again. Press the ESC key twice if you want to abord **Preview**. Fig. 6.14 shows a 3D-view of pathlines.
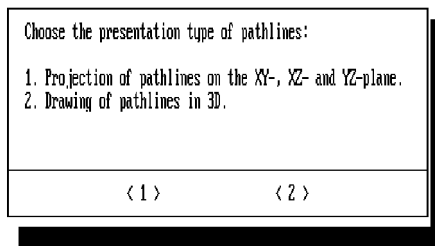

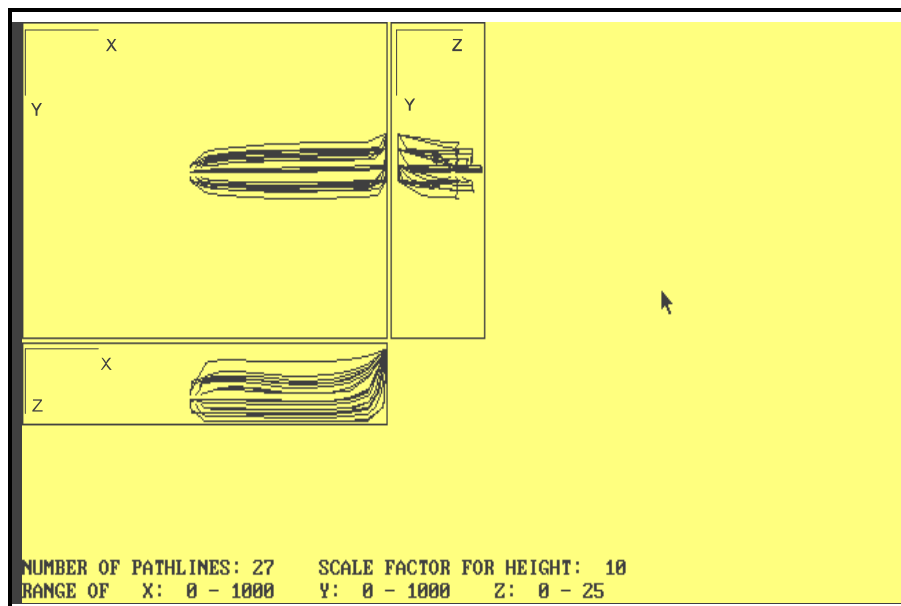Fig. 6.11: The presentation type of pathlines

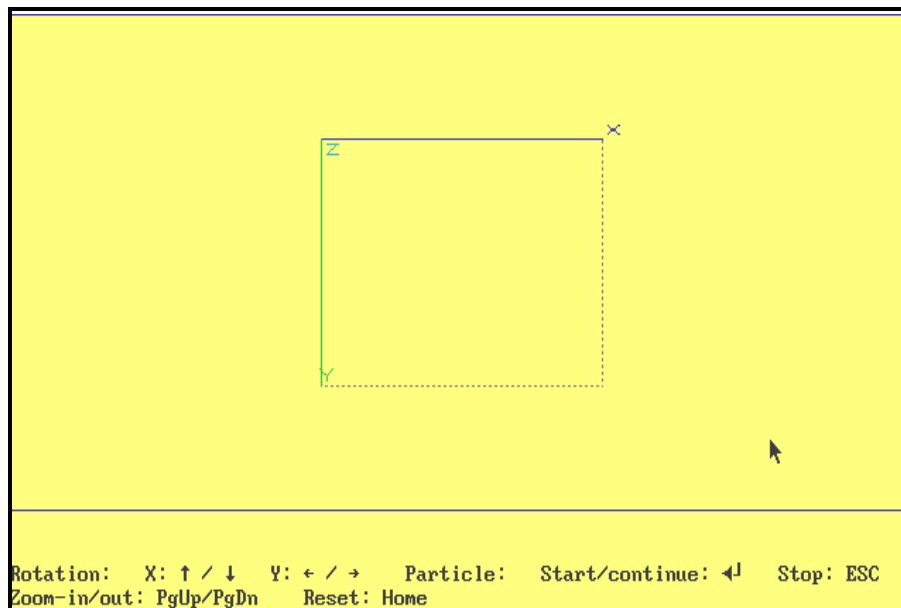Fig. 6.12: Projections of pathlines on the coordinate planes

Fig. 6.13: Using the arrow keys to rotate the model frame
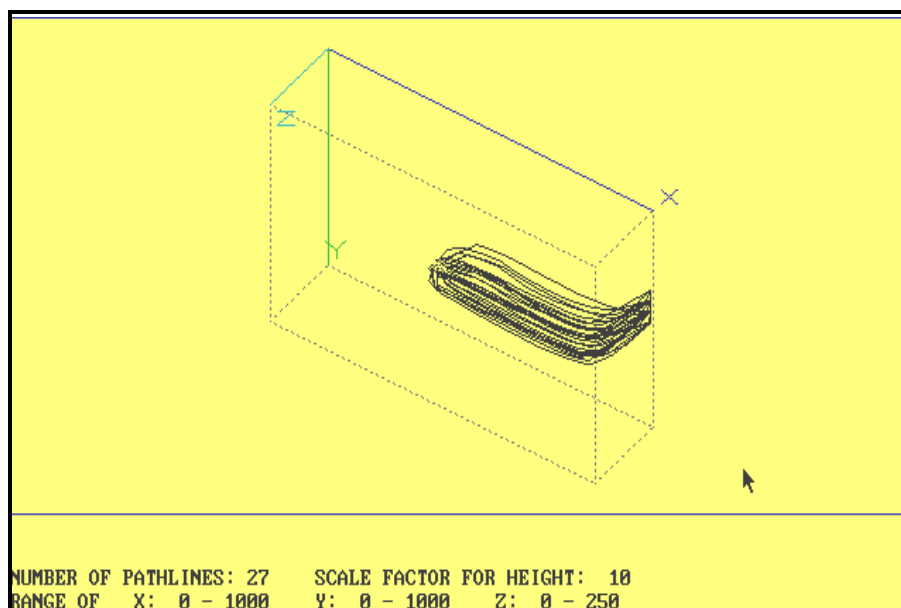
Fig. 6.14: 3D-view of pathlines

HPGL:

Saves the plot in HPGL format. This menu item allows the user to save the projections of pathlines in separate files for each of the coordinate planes. Optionally, a 3D-view can also be saved. The filename and the scale of the plot can be specified in a dialog box.

DXF:

Saves the plot in DXF-format. The filename of the plot can be specified in a dialog box. Optionally, the plot can be output to match the model grid in the map drawn by the user with

PMCAD. Note that only the projection of the pathlines on the XY-plane can be saved in DXF-format.

6.4 Heads-time curves (PMHT)

The program PHMT uses the ASCII file "HEADS.ASC" from a transient simulation to generate temporal development curves of piezometer heads at selected observation points. PMHT has three pull-down menus (Fig. 6.15). The following paragraphs describe the use of each menu item.
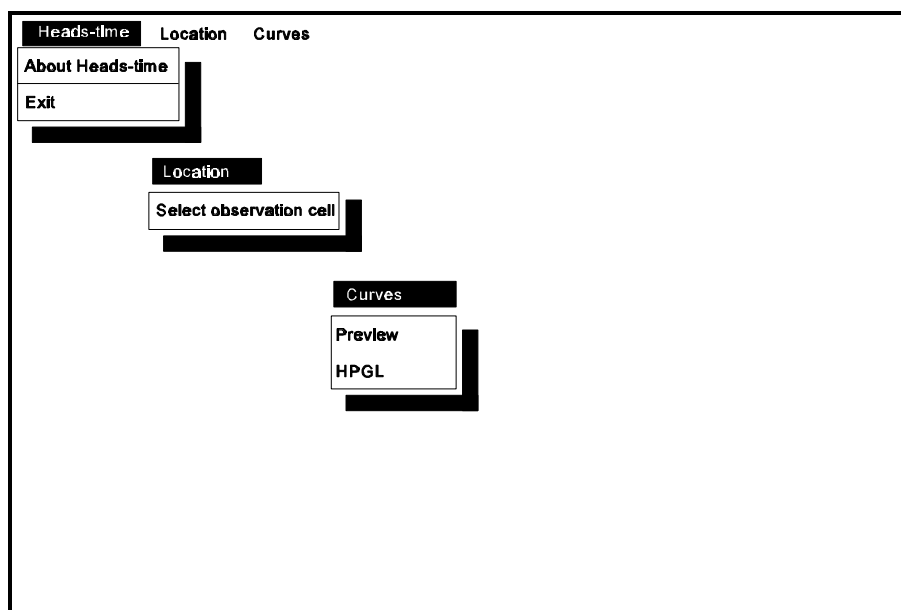
Fig. 6.15: The pull-down menus of PMHT

About Head-time:
Shows the general information about PMHT.

Exit:
Exits PMHT, and returns to the PM-shell.

Select observation cell:
After selecting this menu item, the grid editor will come up. The grid editor is used to locate observation cells by specifying a non-zero value to those cells. PMHT allows a maximum of 10 observation points. If more than 10 points are specified, the supernumerary points are ignored. After having selected the observation cells, PMHT will read the heads from "HEADS.ASC" saved in the data-directory and put the symbol » in the front of this menu item.

Preview:

To show the heads-time curves on the screen, select the menu item "Preview" from the "Curves" menu. PMHT will prompt you to specify the plot parameters. The time axis can optionally be drawn on a linear or logarithmic scale. This menu item cannot be used before the observation cells are specified.

HPGL

This menu item allows the user to save the heads-time curves in HPGL format. This menu item cannot be used before the observation cells are specified.

6.5 Graphic plots (PMGRAF)

The program PMGRAF is called by selecting the menu item "Graphic plots" from the "Analysis" menu of the PM-shell. With this program, all areally-distributed input data, e.g., hydraulic conductivity or concentration, can be displayed in form of contours or classes for each layer. Displaying data in classes means that cells having values within a range are shaded in the same color. The contour level and the range of each class can be specified by the user.

PMGRAF will automatically load the model grid configuration and the boundary conditions of the flow model (IBOUND array) from the model data files specified by using PREMOD. The graphic plots can be used for presentation or data controlling purposes. PMGRAF can also read the ASCII concentration files created by **MT3DCNV** (see section 5.3) and other data files as long as the data file is saved in the format described in Appendix E. The following paragraphs describe the use of the pull-down menus of PMGRAF (Fig. 6.16).

About Graphics:

Shows the general information about PMGRAF.

Exit:

Exits PMGRAF, and returns to the PM-shell.

Menu items of the "Data" menu:

The user can load the data into PMGRAF by selecting a corresponding menu item from the "Data" menu. PMGRAF will prompt you to specify the layer number from which the data 1should be loaded. If the data of a parameter is not specified, the corresponding menu item is colored in gray and cannot be used. The menu item "Other data" allows you to load a data file

saved in the format as described in Appendix E. The matrix contained in the data file must have the same dimension as the current model.
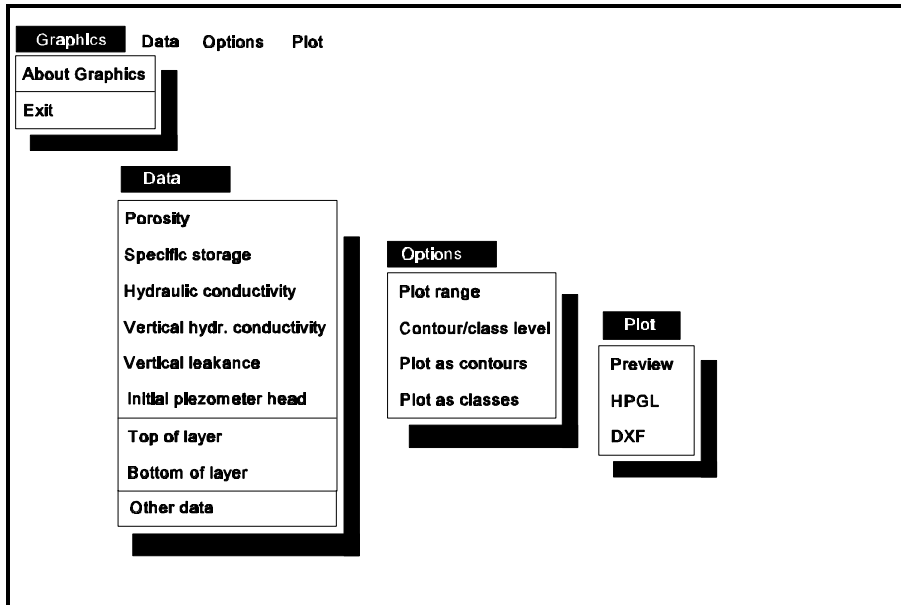
Fig. 6.16: The pull-down menus of PMGRAF

Plot range:

The default plot range is the entire model area. The plot range is defined by the starting and ending column (X) and row (Y) indices in a dialog box (Fig. 6.17). The coordinate system used by the grid editor (see Fig. 4.4) will be used for specifying the indices.
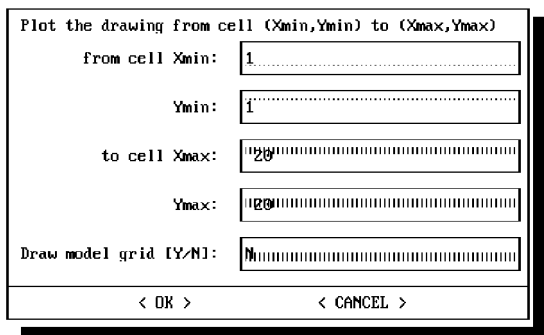
Fig. 6.17: Specification of the plot range

Contour/class levels:

By default, PMGRAF will plot 11 contours from the lower limit to the upper limit of the data. If more than 8 classes are found in the data, PMGRAF will automatically set 8 ranges for the graphics representation. The number of contours or classes and the levels can be changed by selecting this menu item. PMGRAF will prompt you to enter the number of contours or classes. After having enterred the number, you can use the worksheet shown in Fig. 6.18 or 6.19 to

specify the contours levels or the ranges and levels of the classes. The use of the worksheet is described in section 4.2.1.

```
┌─────────────────────────────────────────────────────────────┐
│Specification of contour levels                              │
│┌────────┬──────────┬────────────────────────────────────────┤
││CONTOUR │    LEVEL │                                        │
│├────────┼──────────┤                                        │
││      1 │     .001 │                                        │
││      2 │    .0015 │                                        │
││      3 │     .002 │                                        │
││        │          │                                        │
││        │          │                                        │
││        │          │                                        │
││        │          │                                        │
││        │          │                                        │
│└────────┴──────────┴────────────────────────────────────────┤
│<ENTER>:EDIT  <ESC>:CANCEL  <Alt-Z>:SAVE/EXIT  <PgUp> <PgDn> ↑ ↓ ← →│
│                                                             │
│                                                             │
│                                                             │
│                                                             │
│Model: C:\PM\EX\EXAMPLE                                      │
└─────────────────────────────────────────────────────────────┘
```

Fig. 6.18: Specification of contour levels

```
┌─────────────────────────────────────────────────────────────┐
│Specification of class ranges                                │
│┌────────┬──────────┬──────────┬─────────────────────────────┤
││ CLASS  │     FROM │       TO │                            │
│├────────┼──────────┼──────────┤                            │
││      1 │     .001 │     .001 │                            │
││      2 │    .0015 │    .0015 │                            │
││      3 │     .002 │     .002 │                            │
││        │          │          │                            │
││        │          │          │                            │
││        │          │          │                            │
││        │          │          │                            │
│└────────┴──────────┴──────────┴─────────────────────────────┤
│<ENTER>:EDIT  <ESC>:CANCEL  <Alt-Z>:SAVE/EXIT  <PgUp> <PgDn> ↑ ↓ ← →│
│                                                             │
│                                                             │
│                                                             │
│                                                             │
│Model: C:\PM\EX\EXAMPLE                                      │
└─────────────────────────────────────────────────────────────┘
```

Fig. 6.19: Specification of class ranges

Plot as contours:

Choose this option to make PMGRAF produce contours for the selected data.

Plot as classes:

Choose this option to make PMGRAF produce classes for the selected data.

Preview:

Shows the plot on the screen.

HPGL:

Saves the plot in HPGL-format. PMGRAF will prompt you to enter a filename and the scale of the plot. The default scale is set such that the plot will fit on an A4 sheet (297mm × 210mm).

DXF:

Saves the plot in DXF-format. The plot can be saved to match the model grid of the general map created by using PMCAD. This is done by selecting the option "match the map" in a dialog box as shown in Fig. 6.4.

Appendix A. Application

Appendix A describes the initial and boundary conditions of the sample problem contained in **PM**. The plan view of the model area is illustrated in Fig. A.1. A deposit lies at the central part of the model area. Benzene is dissolved in the groundwater and enters the aquifer system with a concentration equal to 100×10^{-6} kg/m^3 ($=100$ µg/l). A numerical model was developed for this site to calculate the steady-state groundwater flow. Under steady-state flow conditions, the concentration distribution of benzene twenty years after beginning of benzene migration in the aquifer should be calculated.
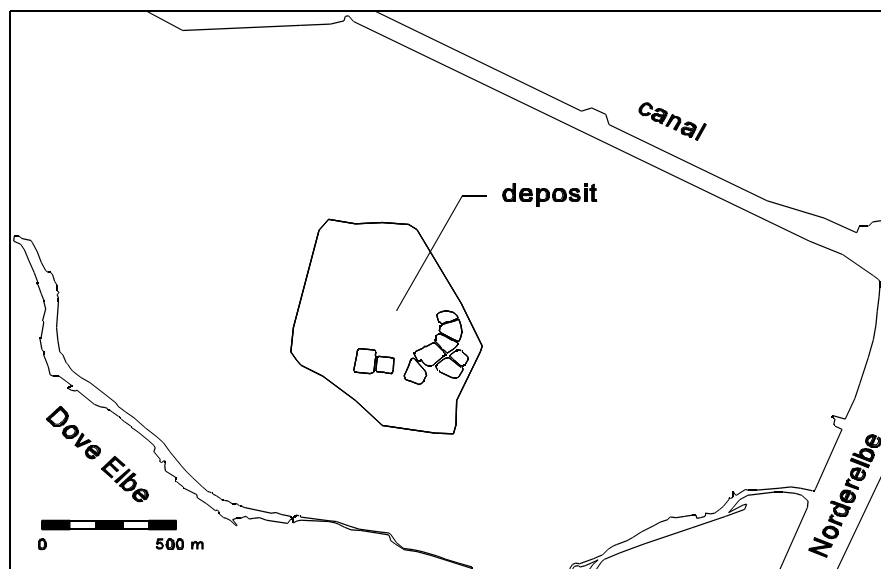

Fig. A.1: Plan view of the model area

The aquifer is discretized into two layers. Both layers are confined. The thickness of the first layer is 8 m and the other 7 m. The discretization of the model area is shown in Fig. A.2, where 55 rows and 57 columns are used. The boundaries of the model area are defined by a canal and the rivers *NORDERELBE* and *DOVE ELBE*. The rivers and the canal are in full hydraulic contact with the aquifer. They can be treated as fixed head boundaries. The other boundaries are defined by stream lines and are therefore impervious (no-flow boundaries). The hydraulic heads in the aquifer at the beginning of the simulation are obtained from a previous flow simulation. The following aquifer parameters and solute properties are assumed constant everywhere:

Effective porosity = 0.2

Horizontal hydraulic conductivity in the second layer = 8.0×10^{-4} m/s

Vertical hydraulic conductivity = 4.0×10^{-5} m/s

Recharge = 2.5×10^{-9} m/s (≈ 80 mm/yr)

Longitudinal dispersivity = 5 m

Distribution coefficient of benzene = 2×10^{-4} m^3/kg

Bulk density of the porous medium in the aquifer = 1700 kg/m^3

Starting concentration = 0 kg/m^3

The ratio of horizontal and vertical transverse to longitudinal dispersivity in both layers is 0.1. The horizontal hydraulic conductivity in the first layer has been specified in the model data. The distribution of this parameter can be displayed by using PMGRAF.
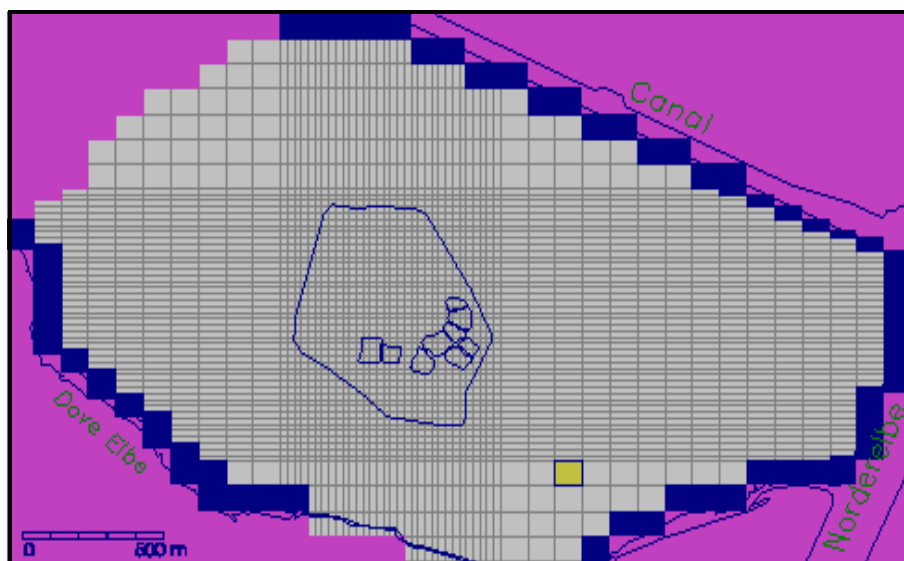

Fig. A.2: Discretization of the model area

Appendix B: Input data files for the simulation models

The input data files created by **PM** for each packages of the simulation models MODFLOW, MODPATH and MT3D are listed below:

MODFLOW:

Basic Package	BAS.DAT
Block-Centered Flow Package (BCF1 or BCF2)	BCF.DAT
River Package	RIV.DAT
Recharge Package	RCH.DAT
Well Package	WEL.DAT
Drain Package	DRN.DAT
Evapotranspiration Package	EVT.DAT
General-Head Boundary Package	BND.DAT
Strongly Implicit Procedure Package (SIP)	SIP.DAT
Slice-Successive Overrelaxation Package (SSOR)	SOR.DAT
Preconditioned Conjugate Gradient 2 Package (PCG2)	PCG2.DAT
Stream-Aquifer Relations Package (STR1)	STR1.DAT
Output Control	OC.DAT

MODPATH and MODPATH-PLOT:

Main data file	MAIN.DAT

(The stress package data files required by MODPATH, such as river or well package are the same as those of MODFLOW.)

MT3D:

Basic Transport Package	BAST.DAT
Advection Package	ADV.DAT
Dispersion Package	DSP.DAT
Sink & Source Mixing Package	SSM.DAT
Chemical Reaction Package	CHE.DAT

Appendix C: Data files used internally by PM

PM saves internally the model data in binary files by using the model name as filename and the extensions given in the following list. The cell-by-cell data files and the zonation data created and used by the grid editor and the zones-editor are indicated by (CBC) and (ZONES), respectively.

Extension   **Description**

ADV   Parameters of the Advection Package used internally by PREMT3D

BOT   Elevation of the bottom of layers (CBC)

BOZ   Elevation of the bottom of layers (ZONES)

CHE   Parameters of the Chemical Reaction Package used internally by PREMT3D

CON   horizontal hydraulic conductivity (CBC)

COZ   horizontal hydraulic conductivity (ZONES)

DPS   Parameters of the Dispersion used internally by PREMT3D

DRC   Hydraulic conductance of the interface between an aquifer and a drain (CBC)

DRE   Elevation of drain (CBC)

DWA   WETDRY array (CBC)

DWZ   WETDRY array (ZONES)

EET   Maximum evapotranspiration rate (volume of water per unit area and unit time (LT^{-1})) (CBC)

EIE   Layer indicator array. For each horizontal location, it indicates the layer from which evapotranspiration is removed (CBC)

ESU   Elevation of the evapotranspiration surface (CBC)

EXD   Evapotranspiration extinction depth (CBC)

FLO   Location of subregions for the computation of water balance (CBC)

GHB   Head on the general-head-boundary (CBC)

GHC   Hydraulic conductance of the interface between the aquifer cell and the general-head boundary (CBC)

HEA   Initial piezometer heads (CBC)

HEZ   Initial piezometer heads (ZONES)

IBD   IBOUND array (CBC)

IBZ   IBOUND array (ZONES)

L   Layer information

LEA   Vertical hydraulic conductivity (CBC)

LEZ   Vertical hydraulic conductivity (ZONES)

LKN   Vertical leakance (CBC)

LKZ   Vertical leakance (ZONES)

LMK   position of model grid and landmarks

MDL   Model information used internally by **PM**

MT3   Menu settings used internally by PREMT3D

OBS   Location of observation cells created and used by PMHT for generating of the heads-time curves (CBC)

POR   Porosity (CBC)

POZ   Porosity (ZONES)

RCD   Information about the location of data arrays

RCH   Recharge flux (LT^{-1}) (CBC)

RCI   Layer indicator array that defines the layer in each vertical column where recharge is applied (CBC)

RIC   Hydraulic conductance of riverbed (CBC)

RIR   Elevation of the bottom of riverbed (CBC)

RIS   Water surface elevation of river (CBC)

SBO   elevation of the bottom of the streambed (CBC)

SCZ   Starting concentration (ZONES)

SEG   sequential number assigned to a group of reaches (STR1 Package) (CBC)

SFL   streamflow in length cubed per time (CBC)

SRE   sequential number of reaches (CBC)

SRO   Manning's roughness coefficient for each stream reach (CBC)

SSL   slope of the stream channel in each reach (CBC)

SST   stream stage (CBC)

STC   streambed hydraulic conductance (CBC)

STO   Specific storage (CBC)

STT   elevation of the top of the streambed (CBC)

STZ   Specific storage (ZONES)

SWI   width of the stream channel in each reach (CBC)

TAL   Longitudinal dispersivity (CBC)

TAZ   Longitudinal dispersivity (ZONES)

TCH   specified concentration of point sources/sinks (constant head, CBC)

TD   specified concentration of point sources/sinks (drain, CBC)

TE   concentration of evapotranspiration flux (CBC)

TG   specified concentration of point sources/sinks (general-head boundary, CBC)

TIC   ICBOUND array (CBC)

TIZ   ICBOUND array (ZONES)

TOP   Elevation of the top of layers (CBC)

TOZ   Elevation of the top of layers (ZONES)

TR   specified concentration of point sources/sinks (river, CBC)

TRA   Time parameters for the flow simulation

TRC   concentration of recharge flux (CBC)

TSC   Starting concentration (CBC)

TSP   Settings of transport steps used internally by PREMT3D

TST   specified concentration of point sources/sinks (stream, CBC)

TW   specified concentration of point sources/sinks (well, CBC)

WEL   Volumetric recharge rate of wells (CBC)

WET   Settings of the BCF2 Package

X   Cell sizes in x-direction

XFD   Settings of import of DXF-maps, this file is internally used by **PM**

Y   Cell sizes in y-direction

Appendix D. Limitations of the preprocessors

The limitations of the preprocesors provided by **PM** are listed below:

The grid editor:

Maximum number of cells in a layer = 15000

Maximum number of cells along columns and rows = 500

Maximum number of layers = 80

Maximum number of stress periods = 1000

There is no limit to the number of wells, general-head boundary cells, rivers and drains.

The zones-editor:

Maximum number of layers = 80

Maximum number of zones in each layer = 20

Maximum number of "connection nodes" of each zone = 40

PMCAD:

Maximum number of user-drawn lines = 5000

Maxinum number of user-drawn circles = 500

Maxinum number of user-drawn arcs = 500

Maxinum number of user-specified text strings = 500

Import of DXF-files:

Up to three DXF-maps can be shown on the screen simultaneously. There is no limit to the size of DXF-background maps. The graphic entities TEXT, LINE, ARC, CIRCLE, POLYLINE (VERTEX) and POINT of the DXF files (version 9.0 or later) can be accepted by **PM**. The other entities are ignored by the program.

Appendix E. Using the grid editor to import/export data

The grid editor allows the user to import/export a two dimensional data array for the layer currently being edited by using the functions **[F9] import** or **Ctrl-[F9] export** (see section 4.1.3). These functions allows the user to read data prepared by the other programs or to transfer parameters between different parameter types. For example, one can save the horizontal hydraulic conductivity in a file and read this data file for assigning the vertical hydraulic conductivity. The export function can also be used for the backup purpose. If it is desired, you can retrieve the data by using the import function.

The following data format is used:
1. Data: NCOL, NROW
2. Data: DATA(NCOL,NROW)

Where NCOL and NROW are the number of columns and rows of the model. DATA() is a two dimensional data array stored row by row. DATA() can be specified in free format. For example, if NCOL=6 and NROW=5, a input file would be:

```
6, 5
0.11 0.12 0.13 0.14 0.15 0.16
0.21 0.22 0.23 0.24 0.25 0.26
0.31 0.32 0.33 0.34 0.35 0.36
0.41 0.42 0.43 0.44 0.45 0.46
0.51 0.52 0.53 0.54 0.55 0.56
```

or

```
6, 5
0.11 0.12 0.13 0.14 0.15 0.16 0.21 0.22 0.23 0.24 0.25 0.26
0.31 0.32 0.33 0.34 0.35 0.36 0.41 0.42 0.43 0.44 0.45 0.46
0.51 0.52 0.53 0.54 0.55 0.56
```

Appendix F: Continuation of a previous run

During a MODFLOW or MT3D simulation, the hydraulic heads or the concentration distribution will be saved in unformatted binary files. Although these files can be directly used for further simulations, the ASCII model files have to be modified by the user.

To solve this problem, the PM-shell will call the conversion programs **PMCNV** and **MT3DCNV** to convert the binary result files into ASCII. Furthermore, the head and concentration distribution in each layer at the last time step will be saved in the files named Hxx or Cxx, where xx is the layer number. PMCNV and MT3DCNV use the data format described in Appendix E to save these files in the data-directory of your model.

The continuation of a previous run in the MODFLOW flow model or in the MT3D transport model is straightforward. First, run PREMOD or PREMT3D and use the grid editor to import the Hxx or Cxx files into the initial heads or the starting concentration. Next, check the time parameters, the data of stress packages and other parameters. Then, select the menu item "Transfer model data" of the "Premod" or "PreMT3D" menu. The ASCII data files for a further simulation are created.

References

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