Processing Modflow X

Version 10.0.23

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Contents

Acknowledgements

We wish to express our sincere gratitude and appreciation to many people who have developed the model codes, Open Source programming libraries, and online resources. This work would not be possible without their generous contributions.

Application and Data Folders

The following folders will be created and used by Processing Modflow.

Application Files
> Per-user installation (with pmx64_10.0.xx.exe or pmx32_10.0.xx.exe):
> C:\Users\YourUserName\AppData\Local\Simcore Software\Processing Modflow 10

> Per-machine installation (with pmx64admin_10.0.xx.exe) for all users:
> C:\Program Files\Simcore Software\Processing Modflow X

> Per-machine installation (with pmx32admin_10.0.xx.exe) for all users:
> C:\Program Files (x86)\Simcore Software\Processing Modflow X

Application Cache and Temporary Files:
> C:\Users\YourUserName\AppData\Simcore Software\Processing Modflow

Examples:
> C:\Users\YourUserName\Documents\My Processing Modflow Models

Abbreviations

CSV File: A comma-separated values file stores tabular data (numbers and text) in plain text. Each line of the file is a data record. Each record consists of one or more fields, separated by commas.

Ctrl-click: Place the mouse pointer to an object; press and hold down the Ctrl key; then press and release the (left) mouse button.

Shift-click: Place the mouse pointer to an object; press and hold down the Shift key; then press and release the (left) mouse button.

Drag and drop or **drag:** Move the mouse pointer to an object; press and hold down the left mouse button; drag the object to the desired location by moving the mouse pointer; then drop the object by releasing the left mouse button.

PM: Processing Modflow.

TOC: The Table of Contents window that is a part of the main window of Processing Modflow X. TOC contains a list of predefined groups; each group may contain user-defined objects.

UTC: Coordinated Universal Time.

UTM: Universal Transverse Mercator.

WGS 84: World Geodetic System 1984**.**

Image of the Start Window

The image of the Start Window of Processing Modflow shows a small section of the expanding remains of a massive star that exploded about 8,000 years ago. Called the Veil Nebula, the debris is one of the best-known supernova remnants, deriving its name from its delicate, draped filamentary structures. The entire nebula is 110 light-years across, covering six full moons on the sky as seen from Earth, and resides about 2,100 light-years away in the constellation Cygnus, the Swan.

Image Credit: NASA/ESA/Hubble Heritage Team. Source: https://www.nasa.gov/image-feature/veil-nebula-supernova-remnant

Supported MODFLOW Packages

BAS6	Basic
BCF6	Block-Centered Flow
CHD	Time Variant Specified Head
DE4	Direct Solver
DIS	Discretization
DRN	Drain
DRT	Drain with Return Flow
EVT	Evapotranspiration
ETS1	Evapotranspiration with a Segmented Function
FHB	Flow and Head Boundary
GHB	General-Head Boundary
GMG	Generic Multigrid Solver
HFB6	Horizontal-Flow Barrier
IBS	Interbed-Storage
LAK	Lake Package
LPF	Layer-Property Flow
LMT7	Flow-Transport Link
MNW1	Multi-Node Well 1
NWT	Newton Solver
OC	Output Control
PCG	Preconditioned Conjugate Gradient Solver
PCGN	PCG Solver with Improved Nonlinear Control
RCH	Recharge
RES1	Reservoir
RIV	River
SFR2	Streamflow-Routing
SIP	Strongly Implicit Procedure Solver
STR	Stream
SUB	Subsidence and Aquifer-System Compaction
SWI2	Seawater Intrusion 2
UPW	Upstream Weighting
UZF1	Unsaturated-Flow
WEL	Well

Variables

HANI   Horizontal anisotropy, dimensionless. HANI x HK = horizontal hydraulic conductivity along model columns.

HK   Horizontal hydraulic conductivity along model rows, in the unit of $[LT^{-1}]$.

m   Thickness of a model layer, in the unit of $[L]$.

ne   Effective porosity, dimensionless.

NCOL   Number of columns of a rectilinear (structured) MODFLOW model grid, dimensionless.

NLAY   Number of layers of a rectilinear (structured) MODFLOW model grid, dimensionless.

NROW   Number of rows of a rectilinear (structured) MODFLOW model grid, dimensionless.

R   Retardation factor [-].

S   Storage coefficient, dimensionless.

Ss   Specific storage, in the unit of $[L^{-1}]$.

Sy   Specific yield, dimensionless.

T   Transmissivity, in the unit of $[L^{2}T^{-1}]$.

VANI   Vertical anisotropy, dimensionless. VANI = HK / VK.

VCONT   Vertical leakance, in the unit of $[T^{-1}]$

VK   Vertical hydraulic conductivity, in the unit of $[LT^{-1}]$.

Chapter 1. Introduction

1.1. What is Processing Modflow

Processing Modflow (PM) was originally developed to support the first official release of MODFLOW (McDonald and Harbaugh, 1988). Since the release of MODFLOW-88, several versions of MODFLOW have been released, such as MODFLOW-96 (Harbaugh, et al., 1996) and MODFLOW-2000 (Harbaugh, et al., 2000), etc. In addition, many model codes have been developed to add functionalities to MODFLOW, for example MODINV (Doherty, 1990) and PEST (Doherty, 2016) enables parameter estimation, MT3DMS (Zheng, et al., 1999) supports the solute transport processes. The list of model codes supported by PM grew over the years.

A decision was made to rewrite PM a few years ago, since some of those supported model codes are no longer maintained by their original authors, and some became obsolete or redundant as they are superseded by newer versions. The present version of PM is the result of the rewrite efforts. The supported model codes have been consolidated and the modeling process has been streamlined with the ability to display model data and results at the same time. As shown in Figure 1, PM comes with a graphical user interface that can display shapefiles and online maps along with the grids and results of multiple models; it can import MODFLOW, MT3DMS (Zheng, et al., 1999), MT3D-USGS (Bedekar, et al., 2016), and SEAWAT (Langevin, et al., 2007) models from their native input data files; it can import model data from various data formats, including
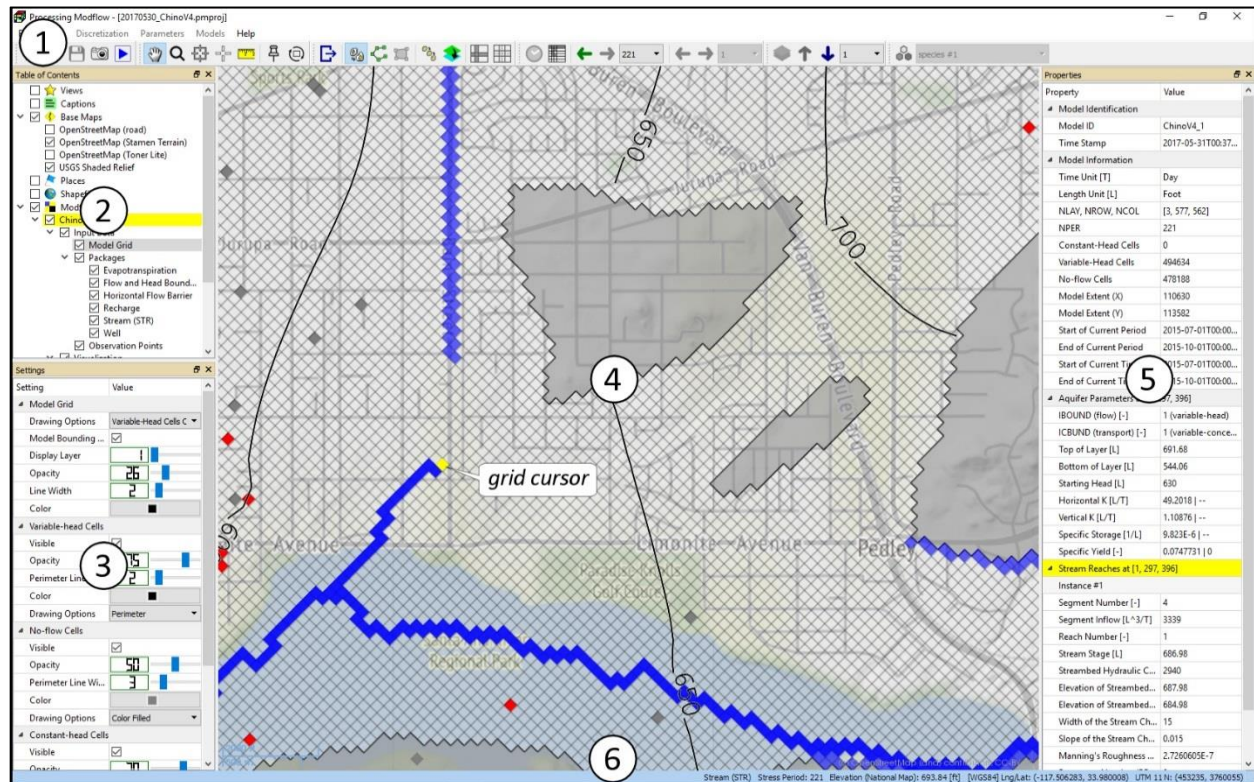

Figure 1. The Main Window of PM

CSV, Shapefile, and ASCII Raster, etc., and it can export model results to raster graphics, shapefiles, charts, and/or text files. The supported model codes are consolidated to the latest official releases of model codes that are actively maintained at the time of writing, including MODFLOW-2005 (Harbaugh, 2005), SEAWAT (Langevin, et al., 2007), MODFLOW-NWT (Niswonger, et al., 2011), MODPATH (Pollock, 2016), MT3D-USGS (Bedekar, et al., 2016), PEST (Doherty, 2016), BeoPEST (Hunt, et al., 2010), and Zone Budget (Harbaugh, 1990). The interface to GSFLOW (Regan, et al., 2018), that couples PRMS (Markstrom, et al., 2015) and MODFLOW-NWT will soon be added.

This text focuses on the use of PM and does not attempt to describe modeling theories or the concept of various packages. Interested users are referred to the user guides of the supported model codes. In addition to the model documents, many groundwater modeling text books are available at nominal cost. For example, (Anderson, et al., 2015) present a comprehensive reference of applied groundwater modeling and (Doherty, 2015) provides the complete theory of calibration and uncertainty analysis.

1.2. Main Window of PM

The main window of PM and its major features are shown in Figure 1. You may use the mouse to drag and rearrange the toolbars, Settings window, and Properties window. A summary of these features is given below.

1. **Menu Bar and Toolbars:**
   - The Menu bar contains several menus that are described in detail in Chapter 3 . We use the notation *Menu > Item* to point to a menu item. For example, *File > Save* means the menu item "Save" of the "File" menu.
   - The File menu is used to save or open PM files, to create or import models, or to save the map in image files. As the Discretization, Parameters, and Models menus only act on the *Active* model (see TOC below), they are activated only if at least one model is loaded under the Models group of TOC.
   - Many model parameters need to be specified during the modeling process. To edit a model parameter, select a corresponding menu item from the Discretization, Parameters, or Models menus. To finish editing, select *Tools > Finish Edit* or click on the ⤷ button on the tool bar.
   - To provide a quick view of the data status, most items of the Discretization, Parameters, and Models menus may be decorated with one of the following icons. A menu item is disabled and greyed out, if it may not be used base on the model configuration.

        ✔   Model data has been specified and will be used in the simulation.

        ▪   Model data has been specified, but will not be used in the simulation.

        No Icon   Model data has not been specified or the item is not associated with an input data, such as *Models > MODFLOW > Run.*

- The toolbar buttons provide shortcuts to some of the menu items. A summary of the toolbar buttons is given in Table 1.
- You may right-click on the area containing the menu bar or toolbars to display a menu that allows for switching on/off toolbars, Settings and Properties windows.

2. **Table of contents Window (TOC)** – The TOC contains a list of predefined groups (e.g. Views, Captions, Images, Base Maps, Shapefiles, and Models). Each group contains a list of items (e.g. maps, shapefiles, models, etc.). And, each item represents a map layer that contains a visual representation of the item's data. When an item is clicked, it is highlighted and becomes the *active layer*. Only one layer can be the active layer at a time. The Settings and Properties windows (see below) displays the settings and values of the active layer. The major functions of the TOC are briefly described below (see the following chapters for more details).

   - Right-click on a group to display a popup menu. This allows the user to add, remove, show, or hide items.
   - Right-click on the Models group to create or import models. When multiple models are loaded in the Models group, only one model can be set as the *Active Model* and the Discretization, Parameters, and Models menus only act on the active model. The active model item is highlighted in yellow on the TOC. Right-clicking on a model item to display a pop-up menu with the following menu items:
      - Set as Active Model[1] – set the model as the active model.
      - Zoom to Model – zoom in to the extent of the model.
      - Remove Model[1] – remove the model and delete its data.

   - Right-click on an item to display a popup menu with item-specific functions, such as Zoom To, Remove Package, Export to Shapefile or Export Matrix Data.
   - The checkbox in front of a group determines whether its items are displayed or hidden.
   - The checkbox in front of an item determines whether it is displayed or hidden. The data of a hidden item remains in the computer's memory. If an item is no longer needed, its removal is recommended.

3. **Settings Window** – This window displays the available visualization settings of the active layer. If a setting contains a text string, double-click on the text string to edit it.

4. **Map Viewer** – This displays base maps, shapefiles, model grid, model cell features, such as wells or stream, and visual representations of model results, such as flow vectors, path lines, head contours, etc.

   - The cell that is pointed to by the *grid cursor* is the *active cell*.
   - You may interact with map with the Pan tool, the Zoom tool, and other tools described in Section 3.5.
   - Many map layers have on-map legends that can be turn on by checking the Visible checkbox in the Settings window of the respective map layer. The captions and the contents of the on-map legends are synced with the TOC with the exception that an

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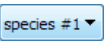
[1] This option is disabled when the Data Editor (Section 3.3.2) or the Grid Editor (Section 3.3.1) is being used.

individual on-map legend can only display up to 40 items. On-map legends can be moved or resized with the mouse. Their positions are anchored on the lower-left corner of the Map Viewer and are therefore independent of the zoom level and position of the map contents.

5. **Properties Window** – This window displays the properties of the selected item of the active layer. For example, if the active layer is a shapefile, this window displays the properties of the selected feature within the shapefile. If the active layer is a model, this window displays the meta data of the model. If a model data, such as Specific Storage, is being edited, this window displays the meta data of the model along with the properties and location of the cell pointed to by the *grid cursor*. The data that is currently being edited is highlighted in yellow. The location of that cell is displayed in the form of [layer, row, column].

6. **Status bar** – This displays the following information

   - The name of the model data set or package that is being edited. For example, *Specific Yield* or *Drain (DRN)*.
   - Current stress period, if the package that is being edited is time-dependent.
   - Ground surface elevation at the mouse cursor's location on the map. Elevation values are provided for reference purposes only and do not represent precisely measured or surveyed values. The ground surface elevation data is provided in the following manner.
     - o Within most parts of the United States, the elevation data is provided by the Point Query Service (PQS) based on the National Elevation Dataset (Gesch, et al., 2002) of the USGS.
     - o Outside of the United States, the elevation data is provided by (MapQuest).
   - Coordinates at the mouse cursor's location on the map. Coordinates are expressed in the World Geodetic System 1984 (National Imagery and Mapping Agency, 1984) datum. For geographic coordinates, negative values are used for longitudinal coordinates in the western hemisphere and latitudinal coordinates in the southern hemisphere. In addition to the geographic coordinates, the Universal Transverse Mercator (Defense Mapping Agency, 1989) coordinates are displayed. The format of the display is "UTM zone Hemisphere: (x, y)," where zone is the zone number of the UTM system ranging from 1 to 60 and Hemisphere is either "N" for North or "S" for South. The coordinates are given as x and y.
   - Layer, Row, Column of the active model at the mouse cursor location.

Table 1. The tool bar buttons

Button	Description
	Start a new PM session.
	Open an existing PM session from a previously saved PM file with the extension ". PMPROJ"
	Save the currently opened PM file. For a new session, the user will be asked to select a new PM file.
	Save the map as an image file.
	Open an Animation dialog box for creating animation files based on model results.
	Pan Tool. Use this tool to pan, zoom, and move the graphics in the map viewer.
	Zoom Tool. Use this tool to zoom in to an area by dragging a rectangular window on the map viewer.
	Observation Tool. Define observation points by clicking on the map.
	MODPATH Tool. Define particle starting points by clicking on the map. Drags a rectangular window to define multiple starting points within the window. This button is active only when the active layer is a MODPATH instance.
	Measure Tool. Use this tool to measure the distance between two points or along a series of points.
	Row Cross Section Tool. Use this tool to visualize model cross sections and/or to edit model data on the row cross section view.
	Column Cross Section Tool. Use this tool to visualize model cross sections and/or to edit model data on column cross section view.
	Pin Tool. Push down this button to disable map pan and zoom with the mouse.
	Rotation Tool. Push down this button to orient the display of the active model grid horizontally.
	Location Tool. Click this button to open the Locator dialog box that allows you to zoom to a cell or a point.
	Finish editing the current data.
	Remove highlight. Within the data editor (Section 3.3.2), you can double-click on a cell to highlight all other cells that have the same value as the clicked cell. The highlight mask may be set to be cleared automatically (see Preferences in Section 3.4.11). Click this button to clear the highlight mask if it is not cleared automatically.
	Switch to the cell-by-cell input method.
	Switch to the polyline input method.
	Switch to the polygon input method.

Button	Description
	Turn on/off the *Copy Cell Data* function. If this button is depressed, the cell value(s) of the current cell will be copied to all cells passed by the grid cursor.
	Turn on/off the *Copy Layer Data* function. If you move to another layer while this button is depressed, the cell values, polylines, and polygons of the current layer will be copied to the destination layer.
	Turn on/off the *Copy Grid Size* function. If this button is depressed, the column and row width of the current cell will be copied to all cells passed by the grid cursor.
	Turn on/off the *Copy Grid Split Factor* function. If this button is depressed, the column and row split factors of the current cell will be copied to all cells passed by the grid cursor.
	Define the temporal discretization data with the Temporal Discretization dialog box.
	Manage the stress period data with the Stress Period Data dialog box.
	Move to the previous stress period. Alternatively, you can alternatively select a destination period from the dropdown box next to the » button.
	Move to the next stress period. Alternatively, you can alternatively select a destination period from the dropdown box next to this button.
	Move to the previous time step. Alternatively, you can select a destination time step from the dropdown box next to the › button.
	Move to the next time step. Alternatively, you can select a destination time step from the dropdown box next to this button.
	Define the layer properties with the Layer Property dialog box.
	Move to the layer above. Alternatively, you can select a destination from the dropdown box next to the ↓ button.
	Move to the layer below. Alternatively, you can select a destination from the dropdown box next to this button.
	Define the species and other transport parameters with the Transport Settings dialog box.
species #1 ▾	Select a species for which the data should be edited.

Chapter 2. Maps

2.1. Views

As shown in Figure 2, a view is defined by one or more polygons and is a tool to help navigating to certain geographical regions. To use Views, follow the instructions provided below.

1. **To add a view:**

   - Right-click on the Views group on the TOC and select **Add Current View** to add the current map area as a View.

Figure 2. A View shown on the map viewer

   - If a polygon-shapefile is displayed, right-click on a polygon-feature of the shapefile to display a popup menu, and then select **Create View** to create a view based on the selected polygon-feature. If the polygon-feature has several rings (i.e., outer and inner rings; inner rings represent holes within the outer ring), the view will consist of multiple polygons to represent those rings.

2. **To remove views:**

   - To remove a view, right-click on the name of the view on the TOC to display a popup menu, and then select **Remove Item**.

   - To remove all views, right-click on the Views group on the TOC to display a popup menu, and then select **Remove All Items**.

3. **To work with a view:**

   - You can zoom to a view by right-clicking on the name of the view on the TOC to display a popup menu, and then select **Zoom to.**

   - You can export a view a shapefile by right-clicking on the name of the view on the TOC to display a popup menu, and then select **Export to Shapefile.**

   - To modify the shape of a view, simply drag its vertices to desired locations.

   - To move a view to another location, hold the Shift-key while dragging one of its vertices.

- A view has two types of vertices that are differentiated by their sizes and color. When a small gray vertex is dragged, it becomes a big white vertex and two small gray vertices will be added next to it. You can remove a big white vertex (and its neighboring small vertices) by right-clicking on it and then select **Remove Vertex** from the popup menu.
- If a view contains more than one polygon, you can remove a polygon by right-clicking on one of its vertices and then selecting **Remove polygon**.

4. **To customize the display of a view**, click on its name on the TOC, and use its Settings window as described below.
   - **Name:** The text string is the name of the View displayed on the TOC. Double-click the text string to modify.
   - **Opacity:** A view is opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.
   - **Polygon Color:** Use the dropdown box to define the color of the view.
   - **Show Vertices:** Check/uncheck the box to turn on/off the display of vertices of the view. You may turn off the display of vertices to avoid unintentional modifications.

2.2. Captions

Captions are text strings that can be added to the Map Viewer. A caption is anchored on the relative position of the map viewer window.

1. **To add a caption:** Right-click on the Captions group on the TOC and select **Add Caption**.
2. **To remove captions:**
   - To remove a caption, right-click on the name of the view on the TOC to display a popup menu, and then select **Remove Item**.
   - To remove all captions, right-click on the Views group on the TOC to display a popup menu, and then select **Remove All Items**.
3. **To work with a caption:**
   - You can move a caption by dragging it with the mouse.
   - You can resize a caption by dragging its corners or borders with the mouse.
4. **To customize the display of a caption**, click on its name on the TOC and use its Settings window as described below.
   - **Name:** The text string is the name of the Caption displayed on the TOC. Double-click the text string to modify.
   - **Caption Text**: This is the text string of the caption. Double-click the text string to modify. If an active model is present, you can insert the following codes to the text string. When you move across time or between layers, these codes will be replaced by the current data of the active model.

- o **\n** = line separator.
- o **{yyyy}** = year. **{m}** = month. **{d}** = day.
- o **{hh}** = hour. **{mm}** = minute. **{ss}** = second.
- o **{sm}** = short month. **{lm}** = long month.
- o **{p}** = stress period. **{t}** = time step. **{l}** = layer

- **Enable Interaction:** Check this box to allow moving and resizing the caption with the mouse.

- **Opacity:** A caption is opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.

- **Color:** Use the dropdown box to define the color of the caption.

- **Font Family, Font Weight, and Font Style**: These define the font for the caption.

- **Text Alignment**: Use the dropdown box to define the alignment of the text string.

- **Text Shadow:** Check this box to add shadow to the caption.

2.3. Image Overlays

Image files can be added as image overlays to the Map Viewer. An image overlay is anchored on the relative position of the map viewer window.

1. **To add an image overlay:** Right-click on the Image Overlays group on the TOC, select **Add,** and then select an image file from the Open File dialog box.

2. **To remove image overlays:**
   - To remove an image, right-click on the name of the view on the TOC to display a popup menu, and then select **Remove Item**.

   - To remove all images, right-click on the Views group on the TOC to display a popup menu, and then select **Remove All Items**.

3. **To work with an image overlay:**
   - You can move an image by dragging it with the mouse.

   - You can resize an image by dragging its corners or borders with the mouse.

4. **To customize the display of an image overlay**, use its Settings window as described below.
   - **Name:** The text string is the name of the Image Overlay displayed on the TOC. Double-click the text string to modify.

   - **Enable Interaction:** If this box is checked, you can use the mouse to drag and resize the image.

   - **Opacity:** An image overlay is opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.

2.4. Raster Maps

Image files, such as digital aerial photos, satellite images, or scanned maps, may be geo-referenced and displayed as raster maps (i.e., offline base map) on the Map Viewer.

Figure 3. A raster map with its vertices

1. **To add a raster map:**

   - Right-click on the Raster Maps group on the TOC, and then select **Add** from the popup menu to display the Open File dialog box.

   - In the Open File dialog box, select the desired image file and then click Open to add the selected image to the Map Viewer[2]. If the size of the image exceeds the Raster Map Image Size defined in Preferences dialog box (Figure 26), the image size is scaled down to that defined size.

   - PM supports image files saved in the following formats: Windows Bitmap (.bmp), JPEG (.jpg), Portable Network Graphics (.png), and Tagged Image File Format (.tif). If the optional projection file[3] and world file[4] are available, PM uses the data of those files to geo-reference your raster map. For images saved in the PNG, JPEG, BMP, or TIFF, the extensions of the world file are ".pgw", ".jgw", ".bpw", or ".tfw", respectively. Images that are saved using File > Save Image (Section 3.4.8) can be added as raster maps.

   - As shown in Figure 3, a raster map consists of an image and a polygon with eight vertices along its perimeter.

2. **To work with a raster map:**

   - You can zoom to a raster map by right-clicking on the name of the view on the TOC to display a popup menu, and then select **Zoom to.**

   - To move (translate) a raster map to another location, hold the Shift-key while dragging one of its vertices.

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[2] The contents of the added image are compressed and then embedded in the saved PM (.pmproj) files. This allows you to share .pmproj files with other users without having to send out image files separately.

[3] A projection file, usually with the file extension ".prj", is a plain text file describing the projection using well-known text format. A prj file has the same base filename as the "main" data file.

[4] World files establish an image-to-world transformation that converts the image coordinates to real-world coordinates. See https://www.loc.gov/preservation/digital/formats/fdd/fdd000287.shtml for details.

- To modify the shape of a raster map, drag its vertices to desired locations. Consider using **Georeference** (see below) if you know the coordinates of vertices on the four corners of the raster map.

3. **To customize the display of a raster map**, click on its name on the TOC, and use its Settings window as described below.

   Figure 4. The Settings window for Raster Map

   - **Name:** The text string is the name of the Raster Map displayed on the TOC. Double-click the text string to modify.

   - **Layer**: This is the layer number of the aerial photograph. When multiple layers are displayed in PM, the layers with smaller layer numbers are displayed on top of the map layers with larger layer numbers.

   - **Opacity:** A raster map is opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.

   - **Polygon Color:** Use the dropdown box to define the color of the raster map border.

   - **Show Polygon:** Check/uncheck the box to turn on/off the display of the polygon of the raster map.

   - **Show Vertices:** Check/uncheck the box to turn on/off the display of vertices of the raster map. You may turn off the display of vertices to avoid unintentional modifications.

   - **Georeference**: Click **Edit** to open the Raster Map Georeference dialog box that allows you to edit the coordinates of the four corners of the raster map. The coordinates of these corner vertices are linearly interpolated to the remaining vertices.

   - **Georeference Options:** This dropdown box defines the number of vertices that can be used for georeferencing purposes. If the options "four vertices" or "eight vertices" is selected, the displayed vertices may be dragged to any position allowing you to deform the map. If the (default) option "Two vertices" is selected, you may drag the displayed vertices to any position, but the shape of the displayed map remains rectangular.

2.5. Base Maps

PM can display online maps from various tiled-map service providers. Several default map services are preprogrammed for your convenience, including various OpenStreetMap styles that are described online at http://wiki.openstreetmap.org/wiki/Tiles. You can add additional tiled-map services to PM. Always be sure to read the terms of use of a tiled-map service provider and
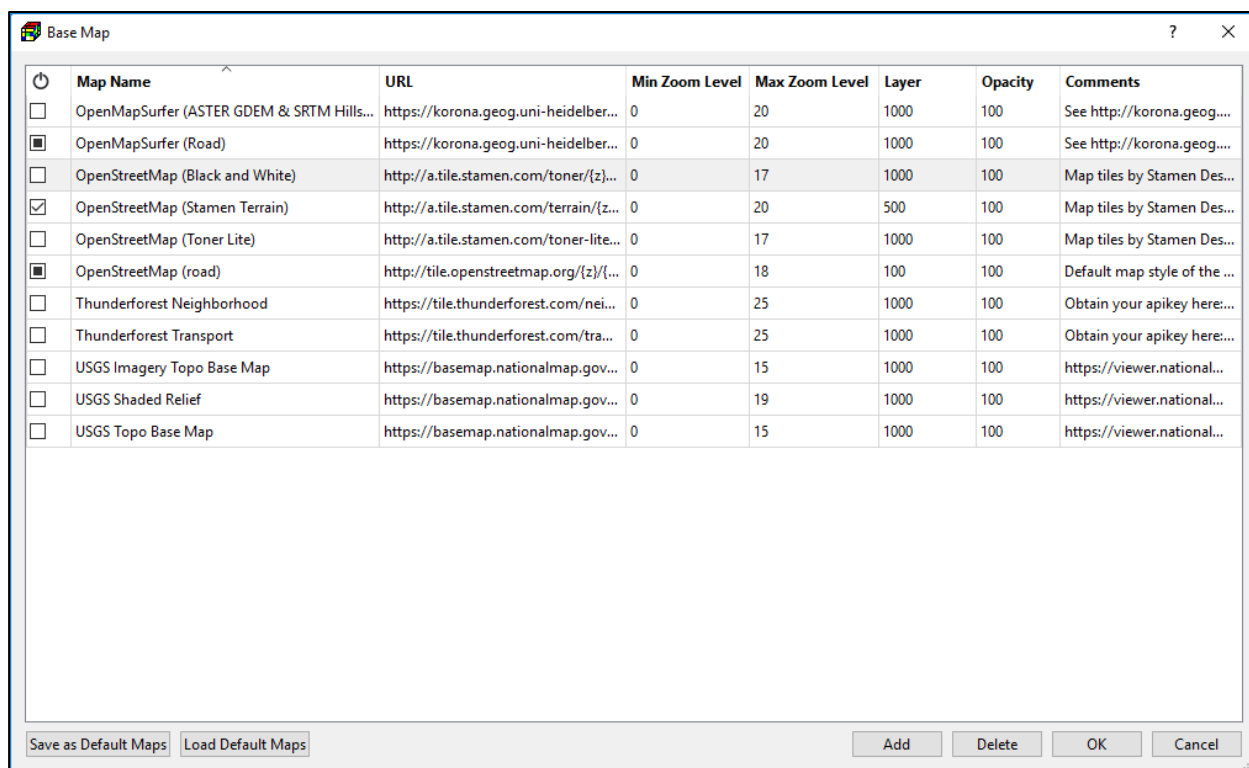
Figure 5. The Base Map dialog box

know its limitations before adding it to PM. The following outlines the procedures for controlling the display of base maps.

2.5.1. Edit Base Maps

To edit the base maps, **r**ight-click on the Base Maps group and then select **Edit Data…** from the popup menu to open the Base Map dialog box (Figure 5). Its features are given as follows.

1. **Table**: The table displays the parameters of tiled-map services that are loaded to the current session. Each row of the table corresponds to a tiled-map service. The columns are

   - ⏻ : Click the checkbox repeatedly to switch between ☑ (checked), ▣ (partially checked), and ☐ (unchecked).

     o Checked ☑: A map item will be added to the TOC and the map item will be checked.

     o Partially Checked ▣ : A map item will be added to the TOC, but the map item will *not* be checked.

     o Unchecked ☐: If the map item representing the corresponding tiled-map service exists on the TOC, the map item will be removed from the TOC.

   - **Map Name** is the name of the Map displayed on the TOC.

- **URL** defines the web address of a tiled-map service and its schema of accessing individual map tiles, such as http://{s}.tile.openstreetmap.org/{z}/{x}/{y}.png**,** where {x}, {y} are placeholders for the tile coordinates, {z} for the zoom level, and {s} is to be randomly replaced by a character a, b, c, or d. Some services use the so-called quadkey (Schwartz, 2010) instead of {x}, {y}, {z} to uniquely identify a single map tile. In that case, use {k} as the placeholder for the quadkey. Some map services require additional parameters, you must add those parameters to the URL accordioning to the requirements of the selected services. A list of tiled-map services and URLs is available here: https://leaflet-extras.github.io/leaflet-providers/preview/

- **Min. Zoom Level/Max. Zoom Level**: These define the available resolutions of a base map. Zoom level 0 encompasses the entire earth; each succeeding zoom level doubles the precision in both horizontal and vertical dimensions. Most maps have a minimum zoom level of 0 and a maximum zoom level between 15 and 21.

- **Layer:** This is the layer number of the base map. When multiple layers are displayed, the layers with smaller layer numbers are displayed on top of the layers with larger layer numbers.

- **Opacity:** A base map is opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.

- **Comments:** A place for additional information of the map or credits to the service provider.

2. **Add:** Click this button to open the Custom Base Map dialog box (Figure 6) that allows you to add a tiled-map service.

3. **Delete:** Click this button to delete the selected row from the table.

4. **Save as Default Maps:** Click this button to save the contents of the table as the default map settings for new PM session.

5. **Load Default Maps:** Click this button to load the previously saved default map settings to the table.

Figure 6. The Custom Base Map dialog box

6. **OK:** Click this button to close the Base Map window. The map items on the TOC will be updated according to the table settings and the map will be displayed on the Map Viewer of the Main Window (Figure 1).

2.5.2. Customize the Display of a Base Map

When selected as the active layer, a base map can be modified in its Settings window. The fields in the Settings window are listed below.

1. **General group**

   - **Name:** The text string is the name of the Map displayed on the TOC. Double-click the text string to modify.

   - **Opacity**: A base map is opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.

   - **Layer:** This is the layer number of the base map. When multiple layers are displayed, the layers with smaller layer numbers are displayed on top of the layers with larger layer numbers.

   - **Min./Max. Zoom Level:** These define the available resolutions of a base map. Zoom level 0 encompasses the entire earth; each succeeding zoom level doubles the precision in both horizontal and vertical dimensions. Most maps have a minimum zoom level of 0 and a maximum zoom level between 15 and 21.

2.6. Shapefiles

The shapefile[5] format (ESRI, 1998) is a geospatial vector format describing spatial features such as points, polylines, and polygons. Each spatial feature is associated with attributes, such as name or temperature. The shapefile format consists of a collection of files with a common base filename with various file extensions, stored in the same directory. Shapefiles may be displayed on the Map Viewer for referencing purposes. Attributes of shapefile polygon features may be imported to model cells directly (See Section 3.5 for details).

When using a shapefile within PM, the files with the following extensions are mandatory:

1. .shp – contains the geometry of spatial features.
2. .dbf – contains the attributes of each spatial features.
3. .prj – contains the coordinate system and projection information.
4. .shx – contains index of the spatial features. It allows fast forward and backward seeking by some software applications. PM does not use this file, but will create it when exporting a shapefile.

2.6.1. Add Shapefiles to the Map Viewer

1. Right-click on the Shapefile group on the TOC, and then select **Add** from the popup menu to display the Open File dialog box.
2. In the Open File dialog box, select the desired shapefile and then click Open to add the selected shapefile to the Map Viewer. Note that the added shapefiles are compressed and then embedded in the saved PM (.pmproj) files. This allows you to share .pmproj files with other users without having to send out shapefiles separately.

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[5] Follow these links SURFER or AutoCAD for details about exporting to shapefile from the respective software.

2.6.2. Customize the Display of a Shapefile

By default, a shapefile is displayed in a single color. To customize the display of a shapefile, use its Settings window and Symbology dialog box as described below.

2.6.2.1. The Settings Window

The following options are available in the Settings window of a shapefile.

1. **General Group**
   - **Name:** The text string is the name of the Shapefile displayed on the TOC and is used as the caption of the on-map legend (see below). Double-click the text string to modify.

   - **Source File:** The text string is the full path of the shapefile. This text string is provided for references purposes and is read-only.

   - **Identify By**: Select a field to be used to identify similar features of a shapefile. When a feature of a shapefile file is clicked, all features of the shapefile with the same value in the selected field are highlighted.

   - **Opacity:** A shapefile is opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.
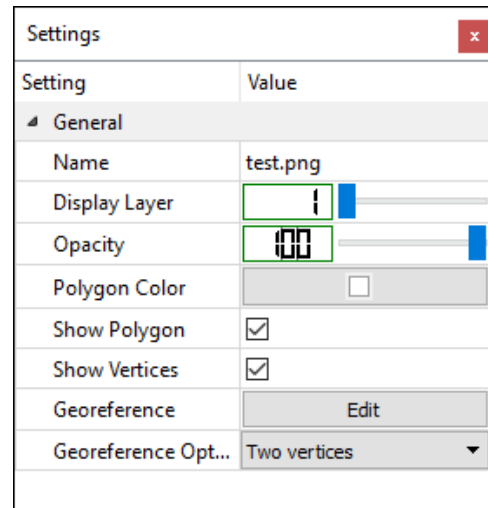
   - **Layer**: This is the layer number of the aerial photograph. When multiple layers are displayed in PM, the layers with smaller layer numbers are displayed on top of the map layers with larger layer numbers.

   - **Line Weight:** This defines the width of displayed line segments in pixels.

   - **Colors**: This displays the color(s) that are currently in use. The colors can be defined using the Symbology dialog box. To open the Symbology dialog box, click on the ⊡ button (The Symbology dialog box is discussed in the following section.)

   - **Pickable:** Check this box to make the shapefile pickable. When a shapefile is pickable, its features may be picked by mouse clicks.

2. **On-map Legend Group**
   - **Visible:** Check this box to display the on-map legend.

   - **Enable Interaction:** If this box is checked, you can use the mouse to drag and resize the on-map legend.

   - **Opacity:** The legend is opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.

   - **Width:** This defines the relative width of the legend. The larger the number the wider is the legend.

   - **Reset Legend:** Click the Reset button to reset the legend to its default size and position.

3. **Label Group**
   - **Visible:** Check this box to display labels.
   - **Field:** This dropdown box contains the attribute fields for the selected shapefile. Use this box to select the field used for labeling displayed shapes.
   - **Display Label:** This dropdown box controls when the labels should be displayed.
   - **Size:** This defines the font size of the labels.
   - **Color:** This defines the color of the labels.

4. **Point Feature Group:** The definitions of this group are ignored if point features are not present in the shapefile.
   - **Type:** This dropdown box defines the shape of point features.
   - **Size**: This dropdown box defines the appearance size of the point features.

5. **Polyline Feature Group:** The definitions of this group are ignored if polyline features are not present in the shapefile.
   - **Label Distance:** This dropdown box adjusts the distance between labels along displayed polylines.

6. **Polygon Feature:** The definitions of this group are ignored if polygon features are not present in the shapefile.
   - **Fill Polygon**: If this box is checked, all polygon features of the loaded shapefile will be filled with the color(s) defined in the Symbology dialog box (see below).

2.6.2.2. The Symbology Dialog Box

Spatial features of a shapefile are associated attribute values. The Symbology dialog box can be used to modify how these values are presented with the spatial features. To open this dialog box, click on the ⊡ button in the Colors field in the Settings window of the shapefile. Three color-mapping styles are available and can be selected using the Style dropdown box:

1. **Single Symbol** (Figure 7)**:** This is the default style and the easiest way to change the color of a shapefile.

   - **Color**: To select a color, click on the ⊡ button in the Symbol group, choose a color from the Select Color dialog box, and click **OK**.

   - **Label:** Enter a label or name for the shapefile and click **OK**. The label will appear in the shapefile legend.
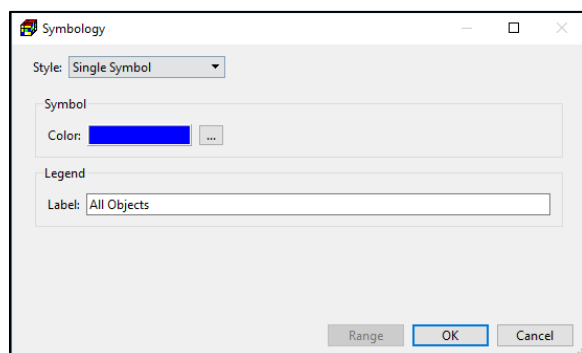
Figure 7. The Symbology dialog box - Single Symbol

2. **Unique Values** (Figure 8)**:** PM can assign a color to each unique value within a selected value field. For example, if a shapefile were to have a value field for land use, a different color could be selected to represent each type of land use (i.e. residential, commercial, agricultural, etc.).
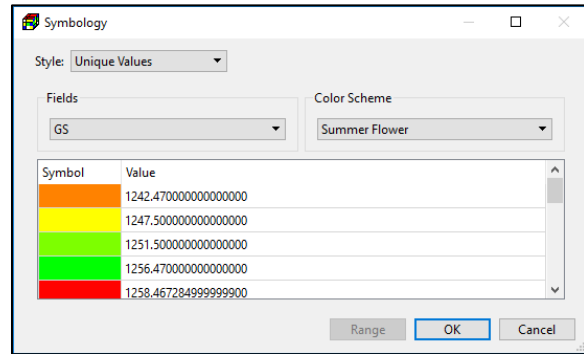
Figure 8. The Symbology dialog box - Unique Values

- **Fields:** This dropdown box contains the value fields for the selected shapefile. Use this box to select a value field.

- **Color Scheme:** This dropdown box contains several pre-defined color schemes. Use this box to select a color scheme.

- **Symbol:** This column displays the colors generated from the selected color scheme. To change a color, double-click on it and choose a new color from the Select Color dialog box.

- **Value:** This column displays the unique values (or strings) of the selected value field. Values cannot be modified.

3. **Graduated Colors** (Figure 9)**:** In this style, the quantitative values of a value field are grouped into classes, and each class is identified by a color. A choropleth map can also be displayed by mapping quantitative values, such as concentration, to a color ramp. For example, darker shades of red could be used to represent higher concentration values and lighter shades could be used to represent lower concentration values. The following describes the options available with the Graduated Colors style:
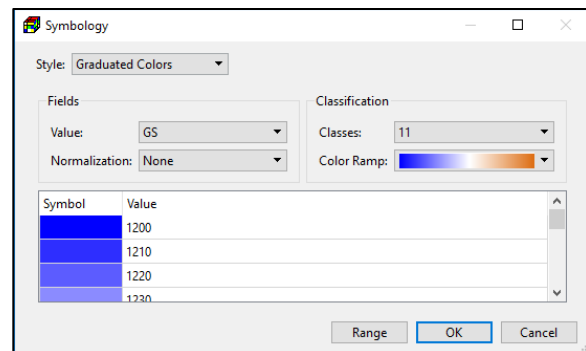
Figure 9. The Symbology dialog box - Graduated Colors

- **Fields Group:** Use the Value dropdown box to select the field that contains the desired quantitative values. Use the Normalization dropdown box to select a field to normalize the data of the Value field. HydroDaVE divides the data of the Value field by the data of the Normalization field and maps the results.

- **Classification Group:** Use the Classes dropdown box to define the desired number of classes to be displayed. Use the Color Ramp dropdown box to assign graduated colors to the classes.

- **Range:** Click this button to specify the lower and upper bounds of the quantitative values to be mapped. The defined range is divided into equal-interval sub-ranges for each class.

- **Symbol:** This column displays the colors of the individual classes. Colors are defined by the selected color ramp. To change a particular color, double-click on the displayed color box and choose a new color from the Select Color dialog box.

- **Value:** This column displays the lower and upper bounds of the individual classes. Values cannot be modified.

Chapter 3. Modeling Environment

3.1. Units

PM requires the use of consistent units throughout the modeling process. For example, if you are using length [L] units of meters and time [T] units of seconds, hydraulic conductivity will be expressed in units of [m/s], pumping rates will be in units of [m³/s] and dispersivity will be in units of [m]. The values of the simulation results are also expressed in the same units. Inconsistent units may be used for concentration values. For example, you may use mg/Liter in a model with the length unit of m. In this case, the calculated concentration will be expressed in mg/Liter and the calculated mass (= volume x concentration) will be expressed in $[m^3 \cdot mg/Liter]$.

Independent of the language and regional settings of your computer, PM always uses period (.) as the decimal point for decimal numerals.

3.2. Temporal Discretization

MODFLOW divides the total time length of a simulation into discrete stress periods, which are, in turn, divided into time steps. The model input parameters are assumed to be constant during a given stress period. For transient flow simulations involving multiple stress periods, the user has the option of changing parameters associated with most flow packages, such as River or Well, from a stress period to another. For transport simulations, the user may change mass-loading rates and source concentrations associated with the fluid sources and sinks.

PM uses the term **Simulation Time**[6] to define a time point in the simulation. **Simulation Time** is the elapsed time (that is given in the consistent time unit, as described in the previous section) since the start of the MODFLOW simulation. Simulation time starts at 0 and increases throughout the course of a MODFLOW simulation.

The numbers of stress periods and time steps as well as the length of the simulation are defined when creating a new model (Section 3.4.6) or importing an existing model (Section 3.4.7). These values can be modified with the Time dialog box. See Section 3.6.1 for details.

3.3. Spatial Discretization

In a MODFLOW model, an aquifer system is represented by a discretized domain consisting of an array of nodes and associated finite difference blocks (model cells). Figure 10 shows the spatial discretization scheme of an aquifer system with a mesh of cells and nodes at which hydraulic heads are calculated. Hydrostratigraphic units can be represented by one or more model layers and the layer thickness may vary from cell to cell. The nodal grid forms the framework of the finite-difference numerical model. Once the head values are computed, they are used to

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[6] Previous versions of PM used the terms "ElapsedTime" or "Elapsed Time".

calculate the cell-by-cell flow terms. The calculated head values and flow terms are the basis for water budget calculation, particle tracking, transport models, and visualization, such as flow vectors and contours.

PM uses the index notation [Layer, Row, Column] to describe the location of a cell in a 3D array. For example, the cell located in the first layer, 6th row, and 2nd column is denoted by [1, 6, 2]. For 2D arrays, the index notation [Row, Column] is used.
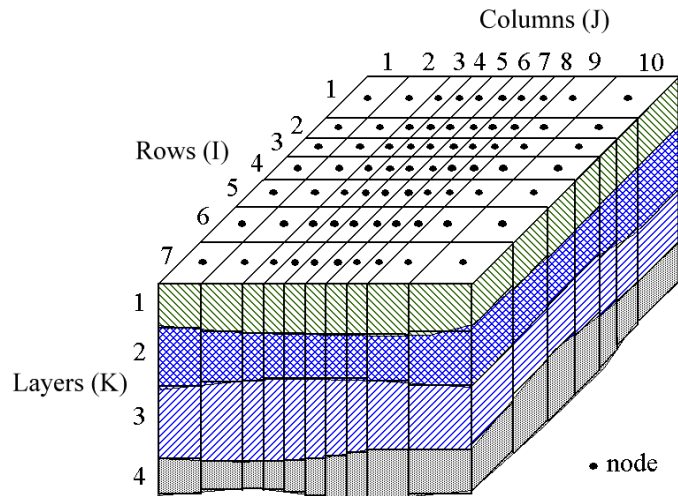
Figure 10. Spatial discretization of a Modflow Model

The numbers of layers, columns, and rows as well as column and row widths are defined when creating a new model (Section 3.4.6) or importing an existing model (Section 3.4.7). These values can be modified with the Grid Editor. See Section 3.3.1 for details.

Model parameters (such as hydraulic conductivity or initial head) and features (such as well or river) are assigned to individual cells with the Data Editor. See Section 3.3.2 for details.

3.3.1. Grid Editor

1. **To start the Grid Editor**, select *Discretization > Grid.* Figure 11 shows the Grid Editor with the grid cursor highlights the entire row and column at the cell location. You may use the Pan tool (Section 3.5.1) and Zoom tool (Section 3.5.2) to interact with the map, to move the grid cursor and/or the model grid.

Figure 11. The Grid Editor with the grid cursor

2. **To modify the column/row width and/or to refine the grid**

- Right-click on the cell where the column/row width or refinement need to be modified or use the arrow keys to move the grid cursor to the cell and then press Enter. The Grid Size dialog box (Figure 12) is displayed.

- Modify the values in the Grid Size dialog box and then click OK to accept the changes.

3. **To end the Grid Editor,** click the ⇥ button on the toolbar or select *Tools > Finish Edit*.

- If changes are made by the Grid Editor, you will be prompted to save or discard the changes.

- If the grid is refined, depending on the nature of the model parameters, they are either kept the same or scaled by the cell size. The following rules apply.
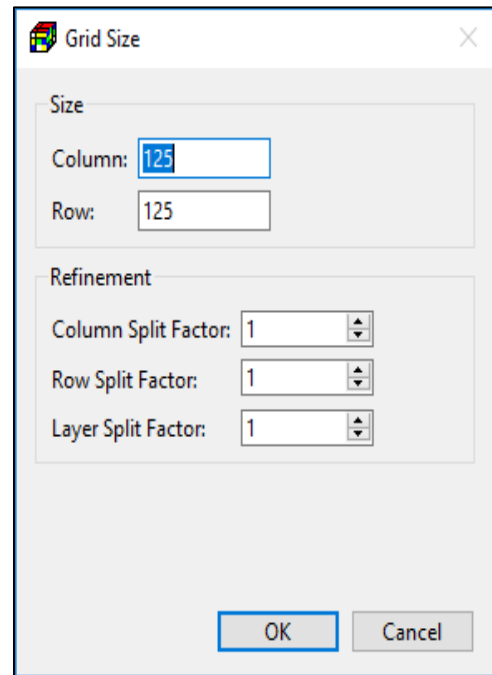
Figure 12. The Grid Size dialog box

  o Pumping rates, mass-loading rate (Section 3.8.3.3.4) and cell-by-cell conductance values of the river, drain, general-head boundary, and stream are scaled by the cell volume. For example, if a well cell is split into to four cells, all four cells will be treated as wells, each with 1/4 of the original pumping rate. The sum of their pumping rates remains the same as that of the previous single well.
  o Transmissivity (T) and storage coefficient (S) values are scaled by the thickness.
  o The parameters of polylines and polygons remain the same, as they are grid-independent. If streams (of the Stream (STR) or the Streamflow-Routing (SFR2) package) have been defined by using the cell-by-cell input method, you must redefine the segment and reach numbers of the streams. For SFR2, you must also redefine the reach length. If streams have been defined by using polylines, you must re-apply polylines to the model cells (see Section 3.3.2.2 for details about the Polyline input method).
  o If an unconfined layer is refined, only the first layer remains unconfined and the others are set as convertible (i.e., convertible between confined and unconfined).
  o All other model parameters remain the same.

3.3.2. Data Editor

The Data Editor is used to assign model parameters, such as HK, VK, drain, well, etc., to individual model cells. The Data Editor provides three input methods for most model parameters. You can use the Cell-by-cell input method to assign values to model cells directly or use the Polyline or

Polygon input methods to help assigning model parameter to model cells. **Regardless of the input methods being used, <u>PM always use the cell-by-cell model parameters in the simulation</u>.**

1. **To start the Data Editor,** select a menu item from the Discretization, Parameters, or Models menu.

2. **To end the Data Editor,** click the ⇨ button on the toolbar or select *Tools > Finish Edit*.

3.3.2.1. Cell-by-Cell Input Method

To activate this input method, select *Tools > Cell-by-Cell Tool* or click the 🖉 button on the toolbar. You can move the *grid cursor* to a cell by dragging the grid cursor, or left-clicking on the cell[7], or using the arrow keys. Table 2 summaries the key assignments and their actions.

Table 2. Key assignments for moving the grid cursor from its current location at [Layer, Row, Column] to the given new location

Key	Action
← (Left)	Move to [Layer, Row, Column - 1]
→ (Right)	Move to [Layer, Row, Column + 1]
↑ (Up)	Move to [Layer, Row - 1, Column]
↓ (Down)	Move to [Layer, Row + 1, Column]
PgUp (page up)	Move to [Layer, Row - 1, Column + 1]
PgDn (page down)	Move to [Layer, Row + 1, Column + 1]
Home (home)	Move to [Layer, Row - 1, Column - 1]
End (end)	Move to [Layer, Row + 1, Column - 1]
Ctrl + ←	Move to [Layer, Row, First Column]
Ctrl + →	Move to [Layer, Row, Last Column]
Ctrl + ↑	Move to [Layer, First Row, Column]
Ctrl + ↓	Move to [Layer, Last Row, Column]
Shift-PgUp	Move to [Layer - 1, Row, Column]
Shift-PgDn	Move to [Layer + 1, Row, Column]
Insert	Highlight cells with the same value (see below)

1. **To assign values to a cell**
   - If the Pan tool (Section 3.5.1) is not activated, activate it by clicking on the 🖐 button on the toolbar or selecting *Tools > Pan Tool.*

   - Right-click on the cell on the Map Viewer to open a dialog box for cell data entry (alternatively, you can move the grid cursor to the desired cell by using the arrow keys or by clicking on the cell, and then press the Enter key to open the dialog box.)

   - In the dialog box, enter new value(s) and then click OK.

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[7] If a pickable shapefile overlies the clicked cell, the shapefile will be picked instead of moving the grid cursor to the cell. To prevent this from happening, uncheck the Pickable box from the Settings window of the shapefile.

- Some packages[8] allows you to assign multiple instances of package-specific features to a cell. For example, you may assign multiple wells to a cell in the Well Package. In that case, the dialog box will include the following functions:

    o *More Actions > Add*: Add a new instance to the current cell.
    o *More Actions > Delete*: Delete current instance from the current cell.
    o *More Actions > Delete All*: Delete all instances from the current cell.
    o Click on ◁ ▷ to go to previous or next instance within the current cell.

2. **To highlight cells with the same value**

- Within the Data Editor, you can double-click on a cell (or press the Insert key) to highlight all other cells that have the same cell value as the clicked cell. The number of highlighted cells will be briefly displayed on the status bar.

- When you are editing the data of a package, you can select a Highlight Parameter from the package's Settings window. The values of the selected Highlight Parameter will be used for highlighting.

- The highlight color changes with repeated double-clicks.

- The highlight opacity may be modified by adjusting the value of *Highlight Opacity* in the Preferences dialog box.

3. To **reset**, **modify**, **import**, and **export** the values of the current layer or the entire model, see the Data menu (Section 3.5.19) for details.

3.3.2.2. Polyline Input Method[9]

To activate this input method, select *Tools > Polyline Tool* or click the ⌇ button on the toolbar. The use of this input method is straightforward. First, you create polylines on the Map Viewer, assign data to one or more vertices of the polylines, and then apply the vertex data to cells along the polylines by means of linear interpolation.

1. **To create/edit polylines**

- If the Pan tool (Section 3.5.1) is not activated, activate it by clicking on the ✋ button on the toolbar or selecting *Tools > Pan Tool*.

- Right-click on the Map Viewer and then select Add Polyline from the popup menu. A polyline will be added to the map (Figure 13). The polyline is centered on the clicked location and stretched to east and west bounds of the current view. The polyline is associated with the current model layer and has three types of vertices that are differentiated by their sizes and color. You may modify the geometry of a polyline by dragging its vertices.

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[8] The following packages allow for assigning multiple instances of package-specific features to a cell: CHD, DRN, DRT1, FHB1, GHB, HFB6, MNW1, RIV, STR, SFR2, and WEL.
[9] The Polyline input method does not support all model parameters/packages. If a model parameter/package is not supported, this method and the ⌇ button are deactivated.

o Model parameter values may be assigned to the big white vertices $\bigcirc$, including the one with the black dot in its center $\odot$, which is the starting point of the polyline. When defining a stream with a polyline, the starting point

Figure 13. A polyline shown on the map viewer

should be placed on the upstream end of the stream.

o You can adjust a polyline by dragging its vertices. The small gray vertices $\bigcirc$ act as "pivot joints" that allow you to modify the shape of the polyline. When a small gray vertex is dragged, it becomes a big white vertex and two small gray vertices will be added next to it.

o You can remove a big white vertex (and its neighboring small vertices) by right-clicking on it and then select **Remove Vertex** from the popup menu.

- You can select a polyline by clicking on one of its vertices. A selected polyline is displayed in yellow and its "big white" vertices are displayed as $\otimes$.

- You can move a polyline with shift-drag. Place the mouse cursor over a vertex, press and hold the left mouse button and Shift-key, move the mouse to drag the polyline, and then release the Shift -key and left mouse button to place the polyline.

2. **To delete polylines**

- To delete a polyline, right-click on a vertex of that polyline to display the popup menu, and then select Delete Polyline.

- To delete all polylines, right-click on a vertex of any polyline to display the popup menu, and then select Delete All Polylines.

3. **To assign data to vertices of polylines**

- If the Pan tool (Section 3.5.1) is not activated, activate it by clicking on the 🖐 button on the toolbar or selecting *Tools > Pan Tool.*

- To display a dialog box for vertex data entry, right-click on the big white vertex where you want to assign data to, then select Edit Vertex Data from the popup menu.

- Enter the data to the dialog box, then click OK. Vertices with specified data are marked with a yellow bracket on the map.

- To clear the specified data of a vertex, right-click on that vertex, and then select Clear Vertex Data from the popup menu.

4. **To apply the vertex data to model cells along polylines**

- Most dialog boxes for the polyline data entry contain » buttons next to the data entry fields. Figure 14, for example, shows the Aquifer Parameter dialog box with the » buttons. You may click the » button next to a parameter to apply its vertex data to the cells along the polyline. For packages[8] that support multiple instances of package-specific features in a cell, such as the Well Package, the » buttons only act on existing instances.
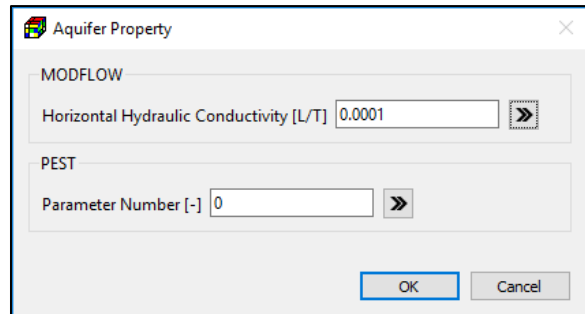
Figure 14. The Aquifer Parameter dialog box

- To apply vertex data of all parameters of a polyline to model cells, right-click on one of its big white vertices, then select *Apply Current Polyline* from the popup menu.

- To apply vertex data of all parameters of all polylines to model cells, right-click on one of the big white vertices, then select *Apply All Polylines* from the popup menu.

- Vertex data are applied to cells with the following rules

  o For cells located between two vertices with data, those vertex data are linearly interpolated to those cells. The distances along the polylines between a cell and those two vertices are used as the weights for linear interpolation.

  o For cells that are not located between vertices with data, the data of the closest vertex is assigned to the cell.

5. **To manage properties of existing polylines:** You can use the Polylines dialog box (Figure 15) to manage the following polyline properties. To open this dialog box, right-click on one of the big white vertices, then select Manage Polylines from the popup menu.

- ⏻: Turn on/off a polyline.
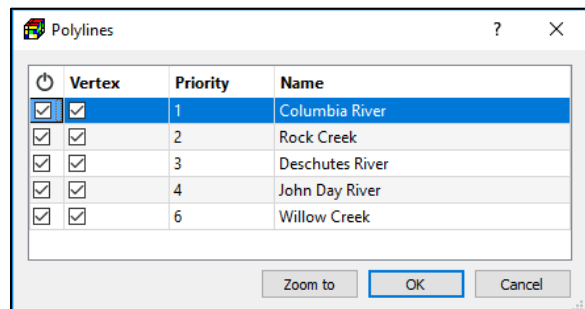
Figure 15. The Polylines dialog box

  o Checked ☑ : Turn on the polyline and display it in the Map Viewer. The vertex data of the polyline may be applied to model cells.

  o Unchecked ☐ : Turn off the polyline. The polyline will not be displayed in the Map Viewer. The vertex data of the polyline may not be applied to model cells.

- **Vertex**: Turn on/off the display of vertices. You may turn off the display of vertices of a polyline to avoid unintentional modifications. The vertex data may still be applied to model cells, even if the display of vertices is turned off.

  o Checked ☑: Turn on the display of the vertices.
  o Unchecked ☐: Turn off the display of the vertices.

- **Priority:** When applying overlapping polylines to cells, the polyline with the smallest priority number has the highest priority.

- **Name:** Name of the polyline.

3.3.2.3. Polygon Input Method[10]

To activate this input method, select *Tools > Polyline Tool* or click the ⬚ button on the toolbar. The use of this input method is straightforward. First, you create polygons on the Map Viewer, assign data to the polygons, and then apply the data to cells lying within the polygons.

1. **To create/edit polygons**

   - If the Pan tool (Section 3.5.1) is not activated, activate it by clicking on the 🖐 button on the toolbar or selecting *Tools > Pan Tool.*

   - Right-click on the Map Viewer and then select Add Polygon from the popup menu. A polygon will be added to the map (Figure 16). The polygon has two types of vertices that are differentiated by

Figure 16. A Polygon shown on the map viewer

   their sizes and color. You may modify the geometry of a polygon by dragging its vertices.

   o You can adjust a polygon by dragging its vertices. The small gray vertices act as "pivots" that allow you to modify the shape of the polyline. When a small gray vertex is dragged, it becomes a big white vertex and two small gray vertices will be added next to it.

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[10] The Polygon input method does not support all model parameters/packages. If a model parameter/package is not supported, this method and the ⬚ button are deactivated.

o You can remove a big white vertex (and its neighboring small vertices) by right-clicking on it and then select **Remove Vertex** from the popup menu.

- You can select a polygon by clicking on one of its vertices. A selected polygon is displayed in yellow.

- You can move a polygon with shift-drag. Place the mouse cursor over a vertex, press and hold the left mouse button and Shift-key, move the mouse to drag the polygon, and then release the Shift -key and left mouse button to place the polygon.

2. **To delete polygons**

- To delete a polygon, right-click on a vertex of that polygon to display the popup menu, and then select Delete Polygon.

- To delete all polygons, right-click on a vertex of any polygon to display the popup menu, and then select Delete All Polygons.

3. **To assign data to polygons**

- If the Pan tool (Section 3.5.1) is not activated, activate it by clicking on the ✋ button on the toolbar or selecting *Tools > Pan Tool.*

- To display a dialog box for polygon data entry, right-click on a vertex of the polygon to which you want to assign data, then select Edit Polygon Data from the popup menu.

- Enter the data to the dialog box, then click OK.

- To clear the specified data of a polygon, right-click on a vertex of that polygon, and then select Clear Polygon Data from the popup menu.

4. **To apply the polygon data to model cells that are located within polygons**

- Most dialog boxes for the polygon data entry contain ≫ buttons next to the data entry fields. Figure 17, for example, shows the Drain Package dialog box with the ≫ buttons. You may click the ≫ button next to a parameter to replace the data of the cells located within the polygon with that parameter value. <u>For packages[8]</u> <u>that support multiple instances of</u> <u>package-specific features in a cell,</u> <u>such as the Well Package, the</u> ≫ <u>buttons only act on existing instances.</u>
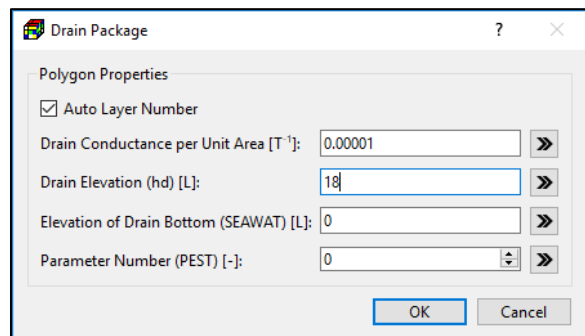
Figure 17. The Drain Package dialog box

- To replace all data of model cells with the data of a polygon, right-click on a vertex of that polygon, then select *Apply Current Polygon[11]* from the popup menu.

---

[11] The priority number or the hole settings (see Figure 18) of that polygon are ignored in this case.

- To replace the data of model cells with the data of <u>all polygons</u>, right-click on the Map Viewer or on one of the vertices, then select *Apply All Polygons* from the popup menu.
- If *Apply Current Polygon* or *Apply All Polygons* contain the following menu item, the final cell values are obtained by the rule of the respective item.

  o **Replace:** Final cell value = polygon value.
  o **Add:** Final cell value = current cell value + polygon value.
  o **Subtract**: Final cell value = current cell value - polygon value.
  o **Multiply:** Final cell value = current cell value × polygon value.
  o **Divide**: For a non-zero polygon value, final cell value = current cell value / polygon value. If the polygon value equals to zero, the cell value remains unchanged.
  o **Minimum:** Final cell value = minimum of the current cell value and the polygon value.
  o **Maximum:** Final cell value = maximum of the current cell value and the polygon value.
  o **Average:** Final cell value = average of the current cell value and the polygon value.

5. **To manage properties of existing polygons:** You can use the Polygons dialog box (Figure 18) to manage the following polygon properties. To open this dialog box, right-click on one of the vertices, then select Manage Polygons from the popup menu.
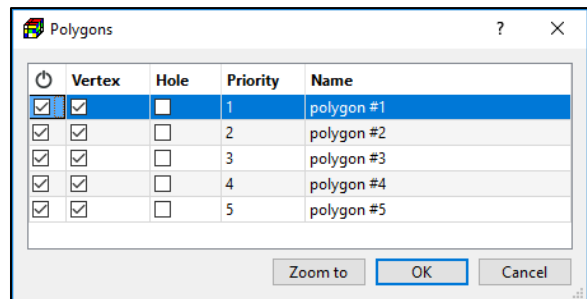
Figure 18. The Polygons dialog box

- ⏻: **Turn on/off a polygon.**

  o **Checked** ☑: Turn on the polygon and display it in the Map Viewer. The data of the polygon may be applied to model cells.
  o **Unchecked** ☐: Turn off the polygon. The polygon will not be displayed in the Map Viewer. The data of the polygon may not be applied to model cells.

- **Hole**: Determines whether a polygon represents a hole.

  o **Checked** ☑: The polygon represents a hole. The data of the polygon may not be applied to model cells.
  o **Unchecked** ☐: The polygon does not represent a hole. The data of the polygon may be applied to model cells.

- **Vertex**: Turn on/off the display of vertices. You may turn off the display of vertices of a polygon to avoid unintentional modifications. The polygon data may still be applied to model cells, even if the display of vertices is turned off.

  o **Checked** ☑: Turn on the display of the vertices.
  o **Unchecked** ☐: Turn off the display of the vertices.

- **Priority:** The priority number is used by the algorithm for applying polygon values to cells using *Apply All Polygons.* For each cell, the algorithm determines the encompassing polygon with the smallest priority number. If that polygon is not a hole, its values are assigned to that cell. If that polygon is a hole or if the cell is not encompassed by polygon, the cell is skipped.

- **Name:** Name of the polygon.

3.3.2.4. Managing Data of Multiple Stress Periods[12]

In MODFLOW, the input data of a given package are assumed to be constant during a stress period and may vary between stress periods. The Stress Period Data dialog box (Figure 19) is designed to manage the data of multiple stress periods. Within the Data Editor, you can open this dialog box by clicking on the ▦ button. The following describes the use of this dialog box.
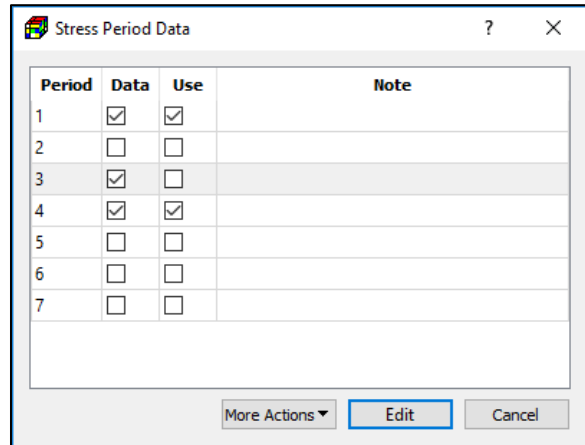
Figure 19. The Stress Period Data dialog box

1. **The Table** displays the status of the model data of individual stress periods.

   - **Data column:**

     o **Checked** ☑**:** Model data has been specified.

     o **Unchecked** ☐**:** Model data has not been specified.

   - **Use column:** A box of this column is activated only if the respective stress period has data. You may check or uncheck the boxes in this column.

     o **Checked** ☑**:** The model data of the respective stress period will be used for the simulation.

     o **Unchecked** ☐**:** The model data from the previous stress period will be used for the simulation.

   - **Note Column:** A place for additional information or notes.

2. **Edit button:** Click to edit the data of the selected period.

3. **Cancel button**: Cancel the changes made to the Use flags and close the dialog.

4. **More Actions:**

   - **Copy:** Select this option to open a Copy Data dialog box that allows you to copy the data from a stress period to another.

---

[12] Data of some packages, such as Horizontal Flow Barriers (HFB6), remain unchanged for the entire simulation. In that case, "Time Independent" will be displayed on the status bar and functions related to multiple stress periods are disabled.

- **Interpolate:** Select this option to open an Interpolate Data dialog box that allows you to linearly interpolate the cell-by-cell data of start and end periods to the periods between them[13]. The model input value changes linearly between specified values based on the simulation times of the stress periods. The interpolated values at the end of stress periods will be used in the model. This Interpolate option is available only if the data that is being edited is one of the following: Recharge (RCH), Evapotranspiration (EVT), Evapotranspiration Segments (ETS1), Unsaturated Zone Flow (UZF1), and concentration data associated with the Sink/Source Mixing (SSM) Package.

- **Delete:** Delete the data of the selected stress period.

Figure 19 shows an example in which the model data for the periods 1, 3, 4 are specified. The specified data of the first period will be used throughout the first three periods. The data of the fourth period will be used for the rest of the simulation. The model data of the third period has been specified but will not be used for the simulation since its Use box is unchecked.

3.4. File Menu

3.4.1. New

Select this menu item to start a new PM session. If changes have been made to the current session, you will be prompted to save the changes to a PM file with the file extension ".pmproj". A PM file contains model data and settings of all graphical objects, except for the model results and online base maps. Links to the model results are stored in the PM file.

3.4.2. Open

This menu item opens an existing PM file[14] in the Open Processing Modflow File dialog box. If changes have been made to the current session, you will be prompted to save the changes to a PM file with the file extension ".pmproj". A PM file contains model data and settings of all graphical objects, except for the model results and online base maps. Links to the model results are stored in the PM file.

3.4.3. Recent Files

This menu allows you to open a PM file from the list of recently accessed files.

---

[13] Linear interpolation applies to floating point values only. For integer values, such as parameter number, the values of the start period apply to all periods between the start and end periods.

[14] A PM file may only be opened by a user at a time. As soon as a PM file is opened, a hidden "lock" file is created to prevent other users from opening the PM file. The lock file is in the same folder as the PM file. The filename of the lock file consists of the filename of the PM file and the string ".~lock~". For example, the lock file for "MyModel.pmproj" is "MyModel.pmproj.~lock~". The lock file will be deleted when the PM file or the application is closed. You may manually delete a lock file, in case it is not deleted correctly.

3.4.4. Save

Select this menu item to save the model data and settings to the currently opened PM file. For a new PM session, you will be asked to select a new PM file from the Save As dialog box.

A backup of the original PM file is created, before it is saved. The filename of a backup file consists of the original filename and the string ".~bak~YYYYMMDDHHMMSS", where YYYY is year, MM is month, DD is day, HH is hour, MM is minute, and SS is second at which the backup file is created. The maximum number of backups is defined in the Preferences dialog box (Section 3.4.11). To restore a backup file, just rename it by removing the string ".~bak~YYYYMMDDHHMMSS".

3.4.5. Save As

Select this menu item to display the Save As dialog box that allows you to save the model data and settings of all graphical objects to a new PM file.

3.4.6. Create Model

This menu item opens the Create Model dialog box (Figure 20) that allows you to create a new model. After a model is created, a model item will be added to the Models group on the TOC. The newly created model will be set as the active model, and the model item will be highlighted in yellow.
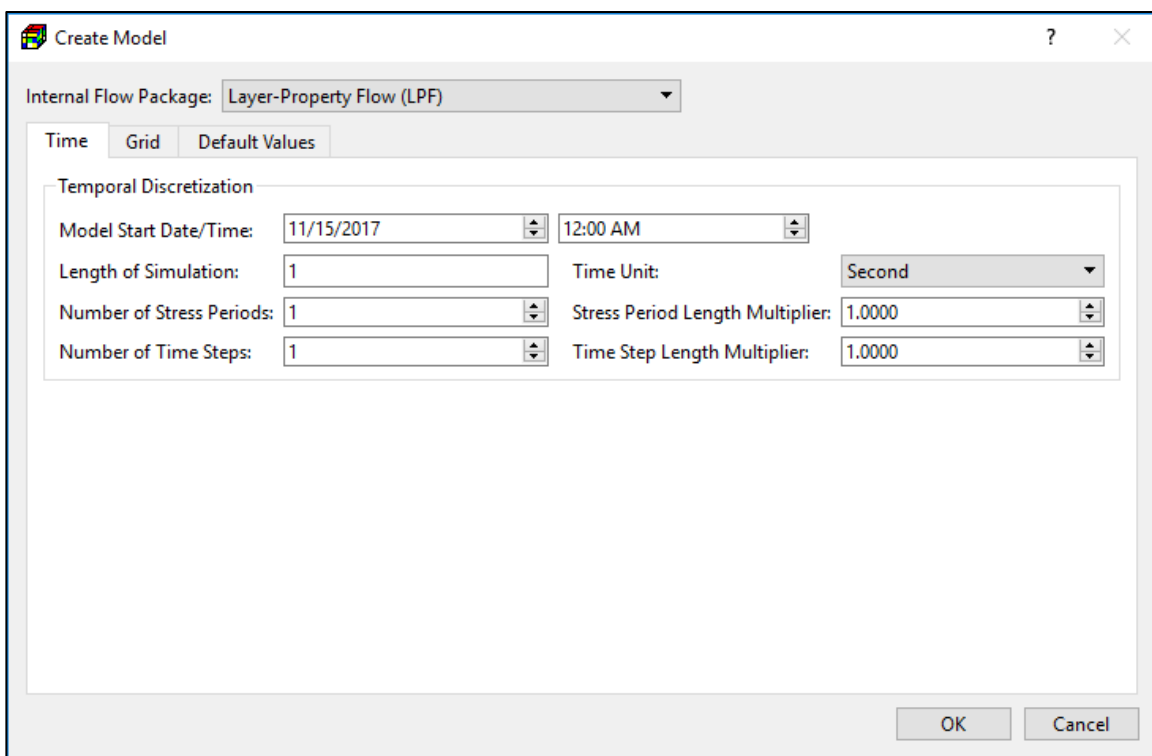
Figure 20 The Create Model dialog box

The features of the Create Model dialog box are discussed below.

1. **Internal Flow Package** is used to specify properties that control groundwater flow between model cells. PM supports three internal flow packages, i.e. the Layer-Property Flow (LPF), Block-Centered Flow (BCF), and Upstream-Weighting (UPW) packages.

   - The LPF and BCF Packages are included in MODFLOW-2005; If LPF or BCF is selected as the internal flow package, the flow simulation will be carried out by MODFLOW-2005 with any of the supported solver packages, but the Newton Solver package.

   - The UPW Package is implemented in MODFLOW-NWT. If UPW is selected as the internal flow package, the flow simulation will be carried out by MODFLOW-NWT with the Newton Solver package. All other solver packages may not be used.

   The UPW Package is designed to solve problems involving drying and rewetting nonlinearities of the unconfined groundwater-flow equation. The LPF and BCF packages use identical conceptualization. The differences between the LPF and BCF packages are primarily in the required input data. You may switch between the supported internal flow packages at any time. See Section 3.6.3 for details about the required input data.

2. **Time Tab** defines the following temporal discretization parameters:

   - **Model Start Date/Time** is the start date/time of the flow simulation.

   - **Length of Simulation** is the length of the flow simulation.

   - **Time Unit** is the time unit of all model data value that involve time.

   - **Number of Stress Periods** is the number of stress periods in the flow simulation.

   - **Stress Period Length Multiplier** is the ratio of the length of each stress period to that of the preceding stress period. The length of the first stress period, ΔT1, is calculated as follows.

$$\Delta T1 = LS \cdot \left(\frac{SPMULT - 1}{SPMULT^{NPER} - 1} \right) \tag{1}$$

   Where LS is the length of simulation, SPMULT is the stress period length multiplier, and NPER is the number of stress periods.

   - **Number of Time Steps** is the number of time steps in each stress period.

   - **Time Step Length Multiplier** is the ratio of the length of each time step to that of the preceding time step. For each stress period, the length of the first time step, Δt1, is related to PERLEN, NSTP, and TSMULT by the relation:

$$\Delta t1 = PERLEN \cdot \left(\frac{TSMULT - 1}{TSMULT^{NSTP} - 1} \right) \tag{2}$$

   Where PERLEN is the length of a stress period, TSMULT is the time step length multiplier, and NSTP is the number of time steps of the stress period.

3. **Grid Tab** defines the following parameters for spatial discretization and georeferenced:

- **Spatial Discretization Group** contains the parameters that defines the extent of the model grid.

  o **Length Unit** is the length unit of all model data values that involve length.
  o **Top Elevation of the Model Grid** will be used as the top elevation of the first model layer.
  o **Number of Rows** is the number of model rows.
  o **Number of Columns** is the number of model columns.
  o **Number of Layers** is the number of model layers.
  o **Total Width of Rows** and **Total Width of Columns** defines the horizontal model extent. The width of individual rows is obtained by dividing the total width of rows by the number of rows. The width of individual columns is obtained by dividing the total width of columns by the number of columns.
  o **Total Thickness of Layers** defines the thickness of the model. The thickness of individual layers is obtained by dividing the total thickness of layers by the number of layers. The layer top elevation and bottom elevation are calculated based on the top elevation of the model grid and the thickness of individual layers. The elevation values may be modified with *Discretization > Layer Top Elevation* and *Discretization > Layer Bottom Elevation.*

- **Georeference Group** contains the parameters that are used to associate the model grid with a spatial location[15].

  o **Georeferencing Method** defines how the model grid is associated with a spatial location.

    – **Latitude/Longitude Coordinates of Grid Corners:** If this method is selected, the user-specified coordinates of the four model grid corners are used to place the model grid on the map.
    – **Grid Azimuth and Coordinates of the Lower-Left Grid Corner:** If this method is selected, the grid azimuth and the coordinates of the lower-left grid corner are used to calculate the coordinates of the remaining grid corners. The result is then used to place the model grid on the map. The **Grid Azimuth** is the angle in degrees measured clockwise from a meridian to the axis along the model's row direction.

  o **Fit to Current View:** Click this button to switch the Georeferencing Method to "Latitude/Longitude Coordinates of Grid Corners" and set the coordinates of the grid corners to fit the current map viewer window.

---

[15] You may subsequently move and/or rotate the model grid with the Pan Tool (Section 3.5.1). The georeference parameters only affect the location and appearance of the model grid on the Map Viewer, i.e., they do not affect the widths of model columns/rows used in the simulation.

4. **Default Values Tab** contains the default values for aquifer parameters. If a required aquifer parameter is not specified, its default value is used in the simulation.

5. **OK:** Click OK to create the model. If the model is created successfully, a model item will be added to the Models group on the TOC and the model item will be highlighted in yellow indicating that the new model is set as the active model. By clicking on the model item, you have access to the Settings window (Figure 21) of the model that includes the following functions.

- **General**

  o **Name:** This text string is the name of the model displayed on the TOC.

  o **Model ID:** This text string is the unique identifier of the model and is used as the name of the subfolder where the generated model input/output files are stored. This subfolder resides in the folder where the PM file is located. If the Model ID is changed, PM will ask whether you want to rename the model's associated subfolder.

  o **Notes**: This is a place for you to write notes about the model. Click the [...] button to open a Model Notes dialog to add or edit notes.

  o **Wrap Arrays:** This setting affects how the model data arrays are written to the model input files. Arrays of all template files for PEST are always written in a wrapped form, even if "do not wrap arrays" is selected. In that case, arrays in templates files are wrapped every 100 columns.
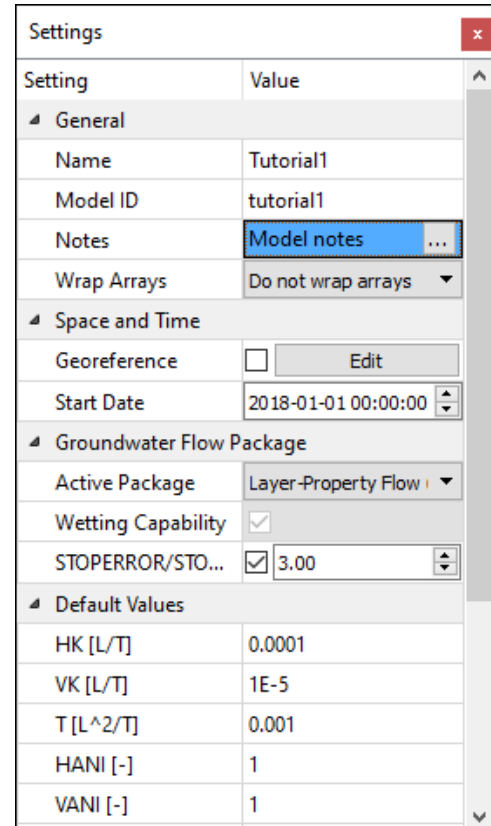
Figure 21. The Settings Window of a model

- **Space and Time**

  o **Georeference:** There are two ways to define the location of the model grid.

    – Click the Edit button to open the Georeference dialog box (Figure 22) that allows you to edit the geo-referencing data. See the Georeference group above for details.

    – Check the checkbox (next to the Edit button) to display a bounding box of the model grid along with four vertices on the corners of the bounding box. You can use the mouse to drag the vertices to desired locations. To move (translate)

the model grid, hold the Shift-key while dragging one of the vertices. To hide the bounding box and its vertices, clear the checkbox.
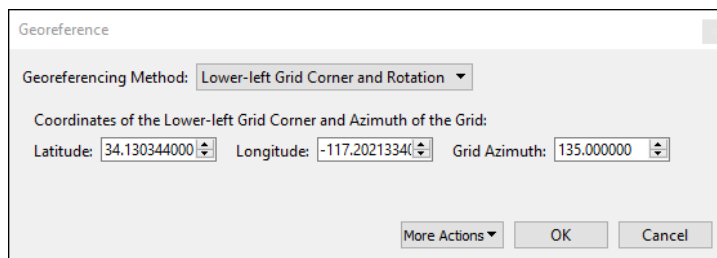
Figure 22. The Georeference dialog box

- o **Start Date** is the start date/time of the flow simulation.

- **Groundwater Flow Package**

  - o **Active Package:** The selected package is used as the internal flow package.
  - o **Wetting Capability**: Check this box to turn on the wetting capability of the BCF or LPF package. See Section 3.8.1.1.21 for details about the wetting threshold and wetting capability of the BCF or LFP package.
  - o **STOPERROR/STOPER**: Check this box to allow the model to continue to the next time step, if it failed to converge and the budget percent discrepancy is less than then given value. If the Upstream Weighting (UPW) Package is selected as the Active Package, this option is disabled. In this case, use the "CONTINUE" option in the Newton Solver (Section 3.8.1.2.6) package instead.

- **Default Values:** If a required aquifer parameter is not specified, its default value is used in the simulation.

3.4.7. Import Model

This menu item opens the Import Model dialog box (Figure 23) that allows you to import an existing MODFLOW model that are stored in the standard format as described in (Harbaugh, et al., 1996), (Harbaugh, et al., 2000) or (Harbaugh, 2005).

The features of the Import Model dialog box are discussed below.

1. **Model Name File:** Click on the ⬚ button and then select a name file from the Open Name File dialog box.

   - PM imports a MODFLOW or a SEAWAT model through a Name File, which specifies the names of the input and output files, associates each file name with a unit number and identifies the packages that will be used in the model. Most packages (except MNW1, OC, SFR2[16], and LMT[17]) of MODFLOW listed in Section 5.2.1 and all packages of MT3D and SEAWAT listed in Sections 5.2.2.1 and 5.2.3.1 may be imported.

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[16] Only input data with the REACHINPUT option activated, NSFRPAR = 0, NPARSEG = 0, ISFROPT = 1 or 3, and ICALC = 0 or 1 are supported. See https://water.usgs.gov/ogw/modflow/MODFLOW-2005-Guide/index.html?sfr.htm for the meaning of those parameters.
[17] Import is not necessary.
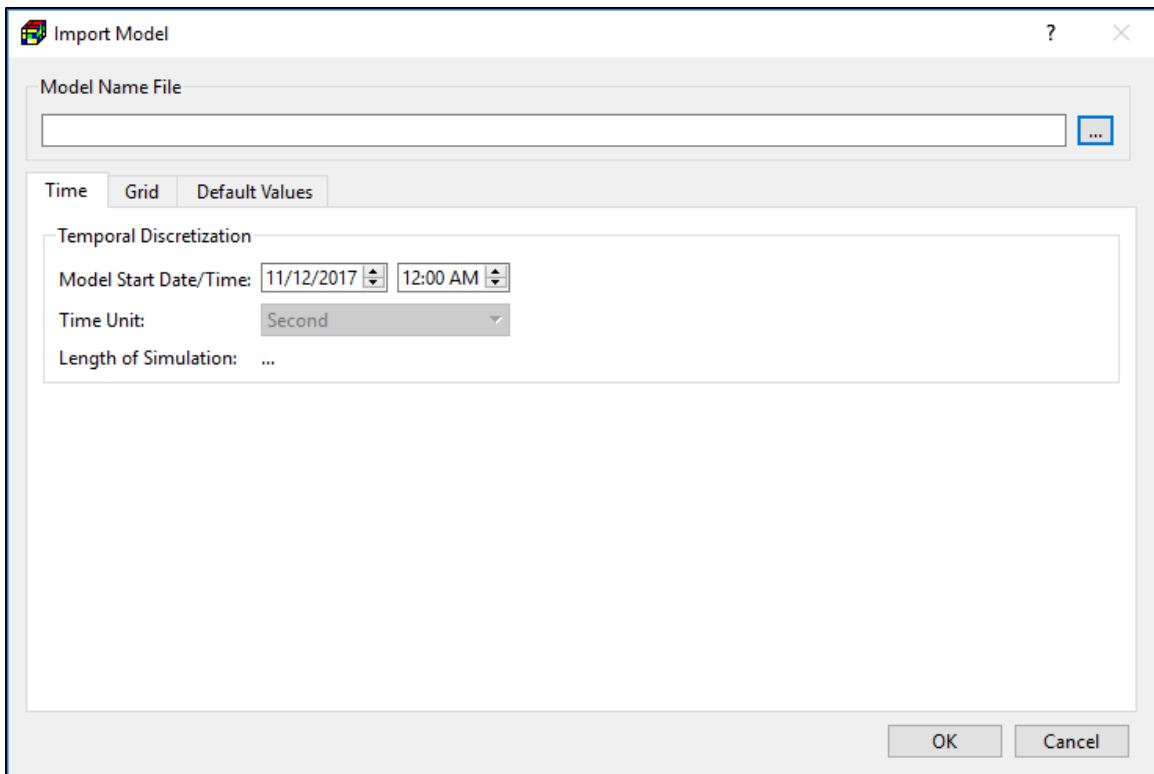
Figure 23 The Import Model dialog box

- To import a MT3D model, you must import the corresponding MODFLOW flow model first, and then subsequently import the MT3D transport model by selecting *Models > MT3D/SEAWAT > Settings*. See Section 3.8.3.1 for details.

2. **Time Tab** defines the following temporal discretization parameters:

   - **Model Start Date/Time** is the start date/time of the flow simulation.

   - **Time Unit** is the time unit of all model data value that involve time. The Time Unit is obtained from the imported model.

   - **Length of Simulation** is the length of the flow simulation of the imported model.

3. **Grid Tab** defines the following parameters for spatial discretization and georeferenced:

   - **Spatial Discretization Group** contains the parameters that defines the extent of the model grid.

     o **Length Unit** is the length unit of all model data values that involve length.
     o **Number of Rows** is the number of model rows.
     o **Number of Columns** is the number of model columns.
     o **Number of Layers** is the number of model layers.
     o **Total Width of Rows** and **Total Width of Columns** defines the horizontal extent of the imported model.

- **Georeference Group** contains the parameters that are used to associate the model grid with a spatial location[15].

  o **Georeferencing Method** defines how the model grid is associated with a spatial location.

    - **Latitude/Longitude Coordinates of Grid Corners:** If this method is selected, the user-specified coordinates of the four model grid corners are used to place the model grid on the map.
    - **Grid Azimuth and Coordinates of the Lower-Left Grid Corner:** If this method is selected, the grid azimuth and the coordinates of the lower-left grid corner are used to calculate the coordinates of the remaining grid corners. The result is then used to place the model grid on the map. The **Grid Azimuth** is the angle in degrees measured clockwise from a meridian to the axis along the model's row direction.

4. **Default Values Tab** contains the default values for aquifer parameters. If a required aquifer parameter is not specified, its default value is used in the simulation.
5. **OK:** Click OK to start the import process. The following actions will be taken during the import process.

   - A model item will be added to the Models group on the TOC. The base filename of the Name file will be used as the name of the model item.

   - A "Model ID" will be assigned to the model item. A subfolder, using the Model ID as its name, will be created in the folder where the PM file is located. All future model input and output files, except the PM file, will be stored in this subfolder.

   - PM will import the input files listed in the Name File. If an input file cannot be found in its given path, PM will search for the input file in the folder where the selected Name File is located. Detailed information about the import process will be stored in the log file "modflow_import_log.txt".

   - If the model import is completed successfully, the model item will be highlighted in yellow indicating that the newly imported model is set as the active model. By clicking on the model item, you have access to the model's Settings windows. See previous section for details.

3.4.8. Save Image

Displays the Save Image dialog box (Figure 24) that allows you to save the map as an image file. Click on the ⬚ button to set the image file name in a Save Image dialog box. Use the Magnification dropdown box to select a magnification factor of the current map. Set a larger value for a higher output resolution[18]. When an image

Figure 24 The Save Image dialog box

file is saved, two additional files with the common base filename and the following extensions are created.

1. .prj – contains the coordinate system and projection information. By default, this file is set to use WGS 1984 World Mercator coordinate system.

2. .pgw, .jgw, or .tfw – contains the World file[4] for the image saved in the PNG, JPEG, or TIFF format, respectively. PM uses WGS 1984 World Mercator coordinate system in the world files.

The saved image files can be used as raster maps, see Section 2.4 for details.

3.4.9. Animation

Displays the Animation dialog box (Figure 25) that allows you to run animations with the model data and optionally save animations into video files or sequences of image files.

1. **Time Control**

   - **Start:** Start date/time of an animation sequence.

   - **End:** End date/time of an animation sequence.

   - **Steps:** Number of animation steps between Start and End. For each step, the corresponding date/time is determined by linear interpolation between Start and End, and then the model results at the date/time are determined and used for visualization with the following rules:
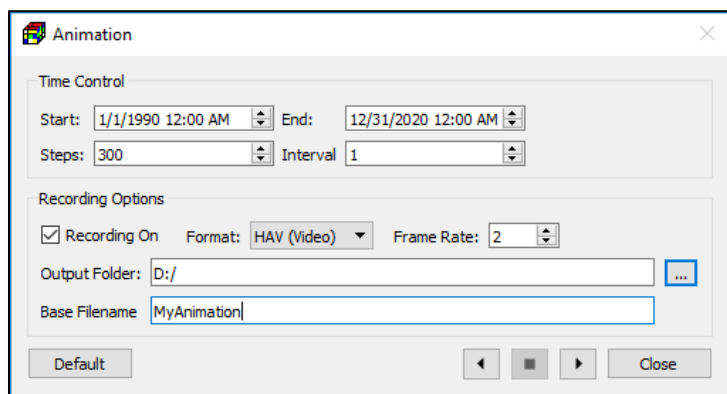
Figure 25 The Animation dialog box

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[18] Setting a higher magnification factor does not change or improve the resolution of the base maps.

o If a step lies before first model result date/time, the first model result will be used for visualization.

o If a step lies after the last model result date/time, the last model result will be used for visualization.

o If a step lies between date/time of two model results, those results will be linearly interpolated to the step. The interpolated values will be used for visualization.

- **Interval:** A video frame is produced when the current animation step is an even multiple of Interval.

2. **Recording Options**

- **Recoding On:** Check this box to turn on recording.

- **Format:** Output format. Select a video format (AVI or HAV) or image format (PNG or JPG). The recorded video frames or images will have the same resolution[19] as the map viewer. AVI is a Microsoft video format that can be played back on most video players. HAV (High quality Audio Video) is a lossless compressed format that can be played back with the free Imagen multimedia player and can be converted to other formats with the VideoMach software. Both software packages are available on www.gromada.com.

- **Frame Rate**: number of frames per second when a recorded video file is played back. The total duration (in seconds) of the recorded video file is approximately Steps/*Interval/Frame Rate*.

- **Output Folder:** click the ⬚ button to select a folder where the video or image files will be saved.

- **Base Filename:** This the base filename (i.e., without a file extension) of output files. The appropriate file extension will be determined based on the selected format, and appended to the base filename.

3. ▶ : Play the animation sequence forwards from *Start* to *End*. Output file(s) will be created or updated if *Recording On* is checked. Make sure that the existing output file(s) are not opened in other applications that may prevent those file(s) from being updated.

4. ◀ : Play the animation sequence backwards from *End* to *Start*. Output file(s) will be created or updated if *Recording On* is checked. Make sure that the existing output file(s) are not opened in other applications that may prevent those file(s) from being updated.

Default: Click this button to set default values to all controls, i.e., *Start* to the model start date/time, *End* to the model end date/time, *Steps* to 10, *Recording* off, *Format* to HAV, *Frame Rate* to 4, etc.

---

[19] It is known that Windows Media Player on Windows 7 or earlier may encounter playback problems with videos that have more than 1080 horizontal lines. It is recommended to resize the Map Viewer to a resolution less than 1080p (i.e., 1920 x 1080) before recording videos. The size of the Map Viewer is displayed on the status bar when resizing the Main Window of PM.

3.4.10. Print

Select this menu item to open the Print dialog box. Its right-hand panel provides a print preview. You can adjust the print settings with the controls on the left-hand panel. Optionally, you can enter a caption and load a logo (saved in the .png or .jpg formats). Click on the Print button on the Top-Left corner of the dialog box to print.

3.4.11. Preferences

Displays the Preferences dialog box (Figure 26) with four tabs as follows.

1. **Path Tab:** This tab contains a table that defines the paths to the executable files of the following supported models and/or applications. When you run a model, PM launches the corresponding executable file. To change the path of a specific model/application, double-click on the respective path and then select an executable file from the *Select Model Executable File* dialog box.

   - **MODFLOW-2005** and **MODFLOW-NWT:**

     o MODFLOW-2005 is a core version of the USGS's three-dimensional (3D) finite-difference groundwater model. For details, visit https://water.usgs.gov/ogw/modflow/index.html.

     o MODFLOW-NWT is a Newton-Raphson formulation for MODFLOW-2005 to improve solution of unconfined groundwater-flow problems. MODFLOW-NWT is

Model	Path
MODFLOW-2005	C:/Program Files/Simcore Software/Processing Modflow X/engine/modflow-nwt/MODFLOW-NWT_64.exe
MODFLOW-NWT	C:/Program Files/Simcore Software/Processing Modflow X/engine/modflow-nwt/MODFLOW-NWT_64.exe
MT3D-USGS	C:/Program Files/Simcore Software/Processing Modflow X/engine/mt3d-usgs/MT3D-USGS_64.exe
MT3DMS	C:/Program Files/Simcore Software/Processing Modflow X/engine/mt3dms/mt3dms5b.exe
SEAWAT V4	C:/Program Files/Simcore Software/Processing Modflow X/engine/seawat/swt_v4x64.exe
PEST	C:/Program Files/Simcore Software/Processing Modflow X/engine/pest/pest.exe
BeoPEST	C:/Program Files/Simcore Software/Processing Modflow X/engine/pest/beopest64.exe
PESTCHEK	C:/Program Files/Simcore Software/Processing Modflow X/engine/pest/pestchek.exe
MODPATH	C:/Program Files/Simcore Software/Processing Modflow X/engine/modpath/mpath7_64.exe
Zone Budget	C:/Program Files/Simcore Software/Processing Modflow X/engine/zonebudget/zonbud.exe
Text Editor	notepad.exe

Figure 26. The Preferences dialog box

a standalone program that is intended for solving problems involving drying and rewetting nonlinearities of the unconfined groundwater-flow equation. For details, visit https://water.usgs.gov/ogw/modflow-nwt/. As MODFLOW-NWT contains several improvements over MODFLOW-2005, the executable of MODFLOW-NWT is assigned to both MODFLOW-2005 and MODFLOW-NWT by default. The executable of MODFLOW-2005 is nevertheless installed on your computer with PM. If desired, you may modify the settings.

- **MT3DMS:** MT3DMS is a modular three-dimensional multispecies transport model for simulation of advection, dispersion and reactions of contaminants in groundwater systems. For details, visit https://hydro.geo.ua.edu/mt3d/index.htm

- **MT3D-USGS:** MT3D-USGS is a USGS updated release of the groundwater solute transport code based on MT3DMS. MT3D-USGS includes new transport modeling capabilities to accommodate flow terms calculated by MODFLOW packages that were previously unsupported by MT3DMS and to provide greater flexibility in the simulation of solute transport and reactive solute transport. For details, visit https://water.usgs.gov/ogw/mt3d-usgs/

- **SEAWAT V4:** SEAWAT is a generic MODFLOW/MT3DMS-based computer program designed to simulate three-dimensional variable-density groundwater flow coupled with multi-species solute and heat transport. The program has been used for a wide variety of groundwater studies including those focused on brine migration in continental aquifers as well as those focused on saltwater intrusion in coastal aquifers. For details, visit https://water.usgs.gov/ogw/seawat/

- **PEST:** This is the standard version of PEST that runs in a single thread. PEST is the industry standard software package for parameter estimation and uncertainty analysis of complex environmental and other computer models. For details, visit http://www.pesthomepage.org/.

- **BeoPEST**: BeoPEST is a special version of Parallel PEST inspired by Beowulf Clusters. A Beowulf Cluster contains several computers that are tied together using a reasonably fast network. When running BeoPEST within PM on a multicore computer, it is configured to run solution agents on individual CPU cores to accelerate the parameter estimation process (by solving the Jacobian matrix parallelly). For details, visit http://www.pesthomepage.org/BEOPEST.php

- **PESTCHEK:** PESTCHEK is a utility program that checks an entire PEST input dataset for correctness and consistency. For details and for additional utilities, visit http://www.pesthomepage.org/PEST_Utilities.php

- **MODPATH:** MODPATH is a particle-tracking post-processing program designed to work with MODFLOW. The included MODPATH version 7 is the fourth major release since its original publication. Note that MODPATH works with MODFLOW-NWT[20]

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[20] For details about the compatibility of MODPATH with MODFLOW-NWT, see this page

provided that the option flag IPHDRY in Models > Modflow > Output Control is checked. For details about MODPATH, visit https://water.usgs.gov/ogw/modpath/

- **Zone Budget:** ZONEBUDGET is a program for computing subregional water budgets for MODFLOW. For details, visit https://water.usgs.gov/nrp/gwsoftware/zonebud3/zonebudget3.html

- **Text Editor**: The text editor is used to display simulation log and certain result files that are saved in the text format. Most text editors, such as NotePad++ or EmEditor, may be used instead of the Windows's default Notepad application.

2. **Visual Tab**

- **Popup Label Color** and **Font Size**: When the mouse hovers over some visual objects, such as flow vectors, their detailed information can be displayed with a pop-up label. The color and font size of the pop-up label are defined here. To change a color, click on the ⬚ button and then pick a color from the Select Color dialog box.

- **Show Scale**: Check this box to display the scale on the lower-left corner of the Map Viewer; clear this box to hide the scale.

- **Background Color**: This defines the background color of the Map Viewer.

- **Ground Surface Elevation Unit**: This defines the unit of the ground surface elevation at the mouse cursor's location on the map. Elevation values are provided for reference purposes only and do not represent precisely measured or surveyed values.

- **Raster Map Image Size**: Size limit of a raster map (Section 2.4) image in mega pixels. If an image exceeds this size, it is scaled down.

- **Use current view as my default view:** Click this button to set the current view extent as the default view extent when PM is started. This button is deactivated when the ⬓ button on the toolbar is depressed.

- **Polyline Opacity** and **Color:** These controls define the color and opacity of polylines created by the Polyline input method (Section 3.3.2.2). The value of opacity ranges from 0 to 100, with 0 being transparent and 100 being opaque.

- **Polygon Opacity** and **Color:** These controls define the color and opacity of polygons created by the Polygon input method (Section 3.3.2.3).

- **Grid Cursor Opacity** and **Color:** These controls define the color and opacity of the grid cursor. For details about the grid cursor, see Sections 0 and 3.3.2.

- **Highlight Opacity** and **Auto Clear:** Within the data editor (Section 3.3.2), you can double-click on a cell to highlight all other cells that have the same value as the clicked cell. The value of Highlight Opacity controls the opacity of the highlight mask. The color of the highlight mask changes with repeated double-clicks. When the **Auto Clear**

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https://water.usgs.gov/water-resources/software/MODPATH/UsingModpathWithModflow-NWT.txt

box is checked, the highlight mask will be cleared automatically whenever the model grid is drawn or redrawn.

- **Value Display Precision:** This is the maximum number of significant digits that is used to display model values on the Properties window.

- **Layer Elevation:** When the top of bottom elevation of a model layer is modified, the elevation of the neighboring layers will be automatically adjusted to match when the **Auto Adjust** box is checked.

3. **Network Proxy Tab**

- **Proxy Type:**

  - **No Proxy**: Choose this if you don't want to use a proxy.
  - **Auto-Detect**: Choose this if you want PM to automatically detect the proxy settings.
  - **Manual**: Choose this if you want to configure the proxy settings manually. PM uses the SOCKS5 protocol to connect to the proxy server.

- **Proxy Settings:** If the selected Proxy Type is *Manual*, you need to provide the proxy server details as follows.

  - **Host**: address of the proxy server
  - **Port**: port of the proxy server
  - **User Name**: user name for proxy authentication
  - **Password**: Password for proxy authentication.

4. **Misc. Tab**

- **Before Running a Model:** Defines the action to be taken before a model run is commenced.

- **After Deleting a Model:** Defines the action to be taken after a model is deleted.

- **PEST Version:** Defines the PEST version to be used for the parameter estimation process.

- **Number of Agents:** This is the number of BeoPEST instances that are used to solve the parameter estimation problem. The default value is the number of physical CPU cores of the computer.

- **Port:** This is the TCP/IP port number that is used by BeoPEST to communicate between the master and agent instances. The port number can be any unused port on the host where the master is run. Port numbers are positive integers between 1024 and 65536. Typically, a port number such as 4004 is unused.

- **Output Width:** This is the output width (in pixels) of charts.

- **Font Size:** This sets the font size of the axis labels and tick labels of charts.

- **Maximum Number of Backups:** This is the maximum number of backups of the currently loaded PM file. A backup is of the loaded PM file is created before it is saved.

- **Start the data editor in the first stress period when editing time-dependent data**: If this check box is checked, the data editor will start in the first stress period when editing time-dependent data/package. If this box is not checked or when editing time-independent data/package, the Data Editor will start in the current stress period.

3.5. Tools Menu

3.5.1. Pan Tool

To activate the Pan Tool, click on the Pan Tool icon 🖐 in the toolbar or select *Tools > Pan Tool.* The Pan tool has the following major functions.

1. **Move the map view in any direction:** Place the mouse cursor within the Map Viewer and drag to move the view. Alternatively, the w, e, d, c, x, z, a, and q keys can be used to move the view towards the north, northeast, east, southeast, south, southwest, west, and northwest, respectively.

2. **Move the grid cursor:**

   - Move the grid cursor to a cell by left-clicking on that cell.

   - Drag the grid cursor with the mouse.

   - Use the arrow keys to move horizontally. Use the Shift-PageUp and Shift-PageDown keys to move to the upper or lower layer.

3. **Move the model grid with shift-drag:** Place the mouse cursor over the grid cursor, press and hold the Shift-key and the left mouse button, move the mouse to drag the model grid, and then release the Shift -key and left mouse button to place the model grid.

4. **Rotate the model grid with ctrl-drag:** Place the mouse cursor over the grid cursor, press and hold the Ctrl-key and left mouse button, move the mouse to rotate the model grid, and then release the Ctrl-key and left mouse button to place the model grid. The center of rotation is the lower-left corner of the unrotated grid.

5. **Zoom in:** Place the mouse cursor within the Map Viewer, press and hold the right button, and move the mouse forward. Release the button when you reach the desired zoom level. Alternatively, if your mouse has a scroll wheel, it can be used to zoom in by scrolling it forward.

6. **Zoom out:** Place the mouse cursor within the Map Viewer, press and hold the right mouse button, and move the mouse backward. Release the button when the desired zoom level is reached. Alternatively, if your mouse has a scroll wheel, it can be used to zoom out by scrolling it backward.

3.5.2. Zoom Tool

To activate the Zoom Tool, click on the Zoom Tool icon 🔍 in the toolbar or select *Tools > Zoom Tool*. The Zoom tool has the following major functions.

1. **Move the map view in any direction:** Press the arrow keys to move the map view toward their respective directions. The w, e, d, c, x, z, a, and q keys can also be used to move the view towards north, northeast, east, southeast, south, southwest, west, and northwest, respectively.

2. **Move the grid cursor** to a desired cell by left-clicking on that cell.

3. **Move the model grid with shift-drag:** Same as the Pan tool described above.

4. **Rotate the model grid with ctrl-drag:** Same as the Pan tool described above.

5. **Zoom in:** To zoom in, position the mouse cursor on the corner of the desired area, press and hold down the left button, drag the mouse cursor to the opposite corner of the desired area, and release the left button. If your mouse has a scroll wheel, it can be used to zoom in by scrolling it forward.

6. **Zoom out:** If your mouse has a scroll wheel, it can be used to zoom out by scrolling it backward.

3.5.3. Observation Tool

The Observation tool is used to define the observation points, and observation values pertaining the observation points. The data can be used by PEST for model calibration or used by the Scatter and Line charts. To activate the Observation Tool, click on the Observation Tool icon ⊞ in the toolbar or select *Tools > Observation Tool.*

1. **Add observation points:** To add observation points to the active model, move to the desired layer with ⬇ or ⬆ buttons on the toolbar and then click on the desired locations on the Map Viewer. The color of the observation points matches with the color assigned to the layer (see Section 3.6.3 for the Layer Properties).

2. **Remove an observation point:** Right-click on the observation point in the Map Viewer to open the Observation dialog box (Figure 27), and then click Delete in the dialog box to delete the selected point.
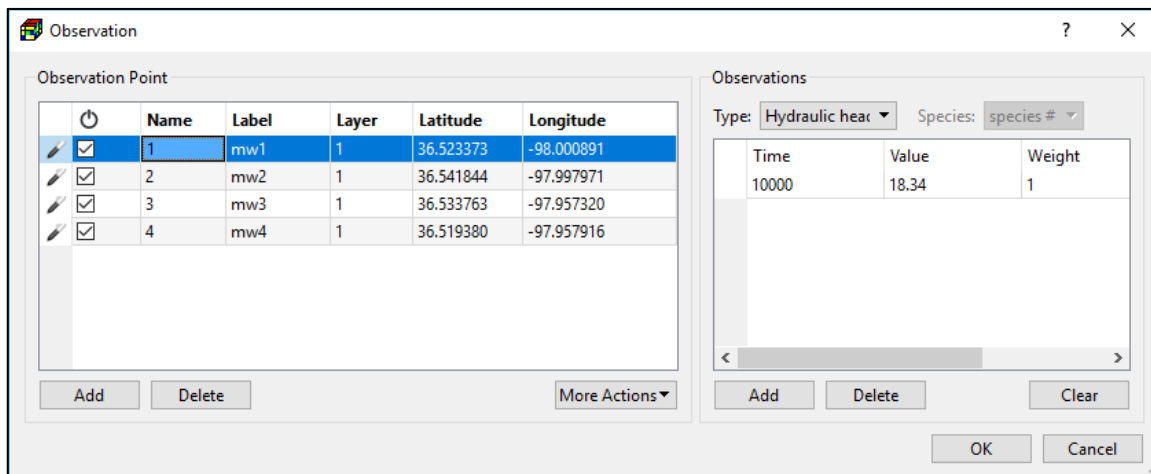
Figure 27. The Observation dialog box

3. **Move observation points:** Place the mouse cursor over an observation point, press and hold the left mouse button, move the mouse to drag the observation point, and then release the left mouse button to place the observation point.

4. **Enter/Edit observation data:** The Observation dialog box (Figure 27) can be used to enter and/or edit observation data. This dialog box can be opened by either right-clicking on an observation point in the Map Viewer or by right-clicking on the Observation Points group on the TOC, and then selecting Edit Data. The features of the dialog box are as follows.

- **Observation Point Group**

  o **Table**: the table displays the observation points and their properties.

    – ⏻**:** Check/uncheck the boxes in this column to turn on/off observation points.
    – **Name**: This column displays the observation point names. The names must be unique.
    – **Label:** This column contains the observation point labels that are displayed next to the observation point on the map. Use "\n" to move to next line; "\u" to move to previous line; and "\\" for backslash. Only ASCII characters with values from 32 to 126 are supported.
    – **Layer**: This column displays the model layer where the observation points are located.
    – **Latitude and Longitude:** These columns display the geographic coordinates (in WGS 84) of the observation points.

  o **Add**: Click this button to add an observation point.
  o **Delete**: Click this button to delete the selected observation points (i.e., rows) from the table[21].
  o **More Actions**

    – **Activate:** Select this option to turn on the selected observation points.
    – **Deactivate:** Select this option to turn off the selected observation points.
    – **Clear**: Select this option to delete all observation points and their associated data.

- **Observations Group:** The controls of this group act on the selected observation point (i.e., the selected row from the Observation Point table).

  o **Type**: This dropdown box is used to select the type of the observation data.
  o **Species**: This This dropdown box is activated only if the Type is Concentration and is used to select the specifies to which the observation data belong.
  o **Table**: The table displays the observation data.

    – **Time**: Observation time, expressed in the simulation time.
    – **Value**: Observed value of the selected Type.

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[21] You may select multiple rows from the table by using combinations of Ctrl-click and Shift-click.

- **Weight**: The Weight of an observation gives a relative confidence level of the observed value. The higher the Weight value, the better is the measurement. The weight can be set at zero if needed (meaning that the observation takes no part in the calculation of the objective function during a parameter estimation process), but it must not be negative. Refer to the PEST User Manual (Doherty, 2016) for the function of weights in the parameter estimation process.

   o **Add**: Click this button to add a row to the Table.
   o **Delete**: Click this button to delete the selected rows from the Table.
   o **Clear**: Click this button to delete all observation data from the Table.

5. **Export/Import observation points:**

   - **Export to Shapefile:** Right-click on the Observation Points group on the TOC, select Export to Shapefile from the popup menu, and then select a shapefile in the Save As dialog box.

   - **Export to Excel File:** Right-click on the Observation Points group on the TOC, select Export to Excel File from the popup menu, and then select an Excel file in the Save As dialog box. The Excel file contains the observation points and observation data. Its format is described in Section 5.1.9.

   - **Import from Excel file:** Right-click on the Observation Points group on the TOC, select Import from Excel File from the popup menu, and then select an Excel file in the Open File dialog box. The Excel file must be saved in the format described in Section 5.1.9. If you need a template file, add at least one observation point to the map and then use the Export to Excel File function to create a template file.

3.5.4. MODPATH Tool

The MODPATH Tool may be accessed only when the active layer is a MODPATH instance. This tool is used to define starting locations for particle tracking. For details of running MODPATH, see Section 4.2.4.

3.5.5. Measure Tool

The Measure tool can be used to measure length of a line or a path. To use this tool, follow the steps provided below.

Figure 28. The Measure Tool

1. Open the Measure Tool (Figure 28) by clicking the ▦ button on the toolbar or selecting **Measure Tool** from the View menu of the Main Window (Figure 1).

2. Position the portion of the map you want to measure within the Map Viewer.

3. Select the Line or Path tab in the Measure tool and click in the Map Viewer to set the beginning point for the line or path. A line consists of two vertices, while a path can consist of two or more vertices. When using the path function, each additional click adds a new vertex. Vertices are displayed as red squares. The length (distance) of the line or path is calculated as the great-circle distance using latitude/longitude coordinates from point to point.

4. Once a line or a path is defined, its shape can be changed by moving its vertices. To move the vertices of a line or path, follow these steps:

   - Activate the defined line or path by selecting the Line or Path tab in the Measure tool. Only one line or path can be made at a time.

   - Mouse over the desired vertex. When the mouse cursor turns into a ☝, click and hold the left button down, move the mouse to drag the vertex to a new position, and release the left button.

   - The length of the line or path is updated while its vertex is being dragged.

5. Click **Clear** to remove the line and path.

6. To close the Measure tool, click the Close button or click the ▥ button on the toolbar.

3.5.6. Row Cross Section Tool

The Row Cross Section Tool (Figure 29) displays the model grid, model features (such as STR or WEL cells), and model results (such as contours, flow vectors and/or pathlines) along a selected model row. The row cross section displays the model columns from the left to the right. The first model column is displayed on the left-hand side of the cross section and the last model column is on the right-hand side. The features of this tool are described as follows.

1. **The Toolbar** contains several buttons and controls as given below.

   🖶 **Print Image.** Click this button to open the Print dialog box that allows you to print the contents of the cross-section window. See Section 3.4.10 for details.

   📷 **Save Image.** Click this button to save the contents of the cross-section window as an image file. See Section 3.4.8 for details.

   ▶ **Animation.** Click this button to open the Animation dialog box that allows you to run animations with the model data and optionally save animations into video files or sequences of image files. See Section 3.4.83.4.9 for details.

   ⚙ **Turn on/off the *Copy Cell Data* function**. If this button is depressed, the cell value(s) of the current cell will be copied to all cells passed by the grid cursor.

   ➦ **Turn on/off the *Copy Slice Data* function**. If you move to another row while this button is depressed, the cell values of the current model row will be copied to the destination row.

   ⛶ **Zoom out to the entire grid**. Click this button to fit the model to the cross-section window.
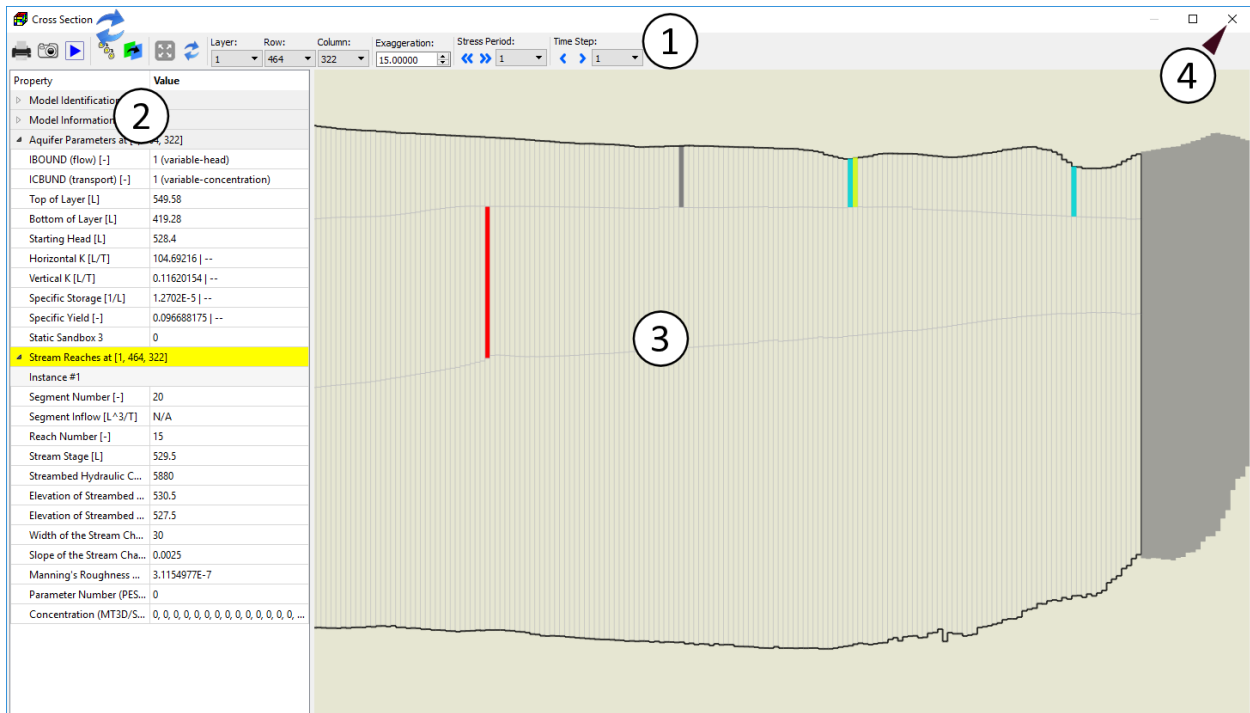
Figure 29. The Row Cross Section Tool

Remove highlight. Within the data editor (Section 3.3.2), you can double-click on a cell to highlight all other cells that have the same value as the clicked cell. The highlight mask may be set to be cleared automatically (see Preferences in Section 3.4.11). Click this button to clear the highlight mask if it is not cleared automatically.

- **Layer/Row/Column:** These dropdown boxes show the numbers of layer, row, and column of the cell pointed to by the grid cursor. You may use these dropdown boxes to move the grid cursor.
- **Exaggeration**: This is the vertical exaggeration factor that is used to adjust the appearance height of the model cross-section.
- **Stress Period:** The dropdown box displays the current stress period. You may use the dropdown box to move to another period. Alternatively, click the « or » button to move to the previous or next stress period, respectively.
- **Time Step:** The dropdown box displays the current time step within the selected Stress Period. You may use the dropdown box to move to another time step. Alternatively, click the ‹ or › button to move to the previous or next time step, respectively.

2. **The Property Window:** This window displays the meta data of the model. If model results are displayed or a model data set is being edited, the properties of the cell pointed to by the *grid cursor* are displayed in this window. The cell data that is currently being edited is highlighted in yellow.

3. **The Cross-Section Window:** This window displays the model grid and model cell features along the model row specified by the **Row** dropdown box. The cell that is pointed to by the *grid cursor* is the *active cell*.

- **Display Settings:** The cross-section window shares the same display settings with the Map Viewer. For example, if contours are displayed on the Map Viewer, they will also be displayed on the cross-section window. See Chapter 4 for details of available display settings.
- **Move the cross-section view in any direction:** Place the mouse cursor within the window and then drag to move the view. Alternatively, the w, e, d, c, x, z, a, and q keys can be used to move the view towards the north, northeast, east, southeast, south, southwest, west, and northwest, respectively.
- **Move the grid cursor.** There are several ways to move the grid cursor.
  - Move the grid cursor to a cell by left-clicking on that cell.
  - Drag the grid cursor with the mouse.
  - Use the arrow keys to move horizontally. Use the Shift-PageUp and Shift-PageDown keys to move to the adjacent rows.
  - Use the Layer/Row/Column dropdown boxes on the toolbar.
- **Zoom in:** Place the mouse cursor within the window, press and hold the right button, and move the mouse forward. Release the button when you reach the desired zoom level. Alternatively, if your mouse has a scroll wheel, it can be used to zoom in by scrolling it forward.
- **Zoom out:** Place the mouse cursor within the window, press and hold the right mouse button, and move the mouse backward. Release the button when the desired zoom level is reached. Alternatively, if your mouse has a scroll wheel, it can be used to zoom out by scrolling it backward.
- **Edit Cell data**: If you invoke the Row Cross-Section Tool while editing a certain model data, you may edit the cell data by right-clicking on the cell of interest. You can double-click on a cell (or press the Insert key) to highlight all other cells that have the same cell value as the clicked cell.

4. **Close the Tool.** To close the tool, click the X button located on its upper-right corner. After closing this tool, the grid cursor on the Map Viewer will be moved to the cell pointed to by the Layer/Row/Column dropdown boxes of this tool. The model on the Map Viewer will be redrawn if necessary.

3.5.7. Column Cross Section Tool

The Column Cross Section Tool displays the model grid, model features (such as STR or WEL cells), and model results (such as contours, flow vectors and/or pathlines) along a selected model column. The column cross section displays the model rows from the left to the right. The first model row is displayed on the left-hand side of the cross section and the last model row is on the right-hand side. See previous section for details about the features of this tool.

3.5.8. Pin Tool

Select *Tools > Pin Tool* or push down the 🖈 button on the toolbar to disable map pan and zoom with the mouse.

3.5.9. Rotation Tool

Select *Tools > Rotation Tool* or push down the ⬚ button on the toolbar to orientate the display of the active model grid horizontally. All other visual objects, including other models, will be rotated with the active model grid accordingly.

3.5.10. Location Tool

Select *Tools > Location Tool* or click the ▶ button on the toolbar to open the Locator dialog box that has two tabs. The Model Cell tab (Figure 31) allows you to locate a model cell, and the Location tab (Figure 31) allows you to pinpoint a location.

1. **To locate a model cell**
   - Click on the Model Cell tab (Figure 31),
   - Enter the row and column of the cell,
   - Click OK to zoom to the model cell. A cross ✛ will be placed in the center of the cell for a short time.

2. **To pinpoint a location**
   - Click the Location tab (Figure 31),
   - Specify the Projection, Datum, and Coordinates of the desired location,
   - Click OK to zoom to the location. A cross ✛ will be placed in the given location for a short time.

3.5.11. Finish Edit

Click on the ⤷ button on the toolbar to finishing editing the grid or the model data. If changes have been made, you will be prompted to save or discard the changes.
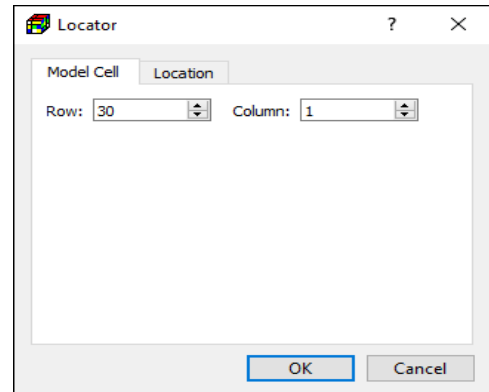
Figure 31. The Model Cell tab of the Locator dialog box
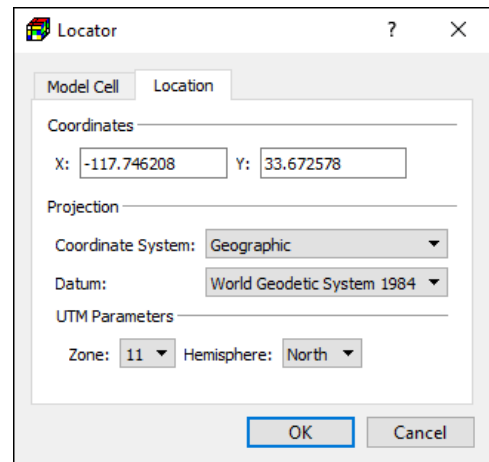
Figure 31. The Location tab of the Locator dialog box

3.5.12. Cell-by-Cell Tool

Within the Data Editor, you may select *Tools > Cell-by-Cell Tool* or push down the ⬚ button on the toolbar to switch to the Cell-by-Cell input method. See section 3.3.2.1 for details.

3.5.13. Polyline Tool

Within the Data Editor, you may select *Tools > Polyline Tool* or push down the ⬚ button on the toolbar to switch to the Polyline input method. See section 3.3.2.2 for details.

3.5.14. Polygon Tool

Within the Data Editor, you may select *Tools > Polygon Tool* or push down the ⬚ button on the toolbar to switch to the Polygon input method. See section 3.3.2.3 for details.

3.5.15. Cell Copy

Within the Data Editor, you may select *Tools > Cell Copy* or push down the ⬚ button on the toolbar to turn on the *Copy Cell Data* function. If this button is depressed, the cell value(s) of the current cell will be copied to all cells passed by the grid cursor.

3.5.16. Layer Copy

Within the Data Editor, you may select *Tools > Layer Copy* or push down the ⬚ button on the toolbar to turn on the *Copy Layer Data* function. If you move to another layer while this button is depressed, the cell values, polylines, and polygons of the current layer will be copied to the destination layer.

3.5.17. Grid Size Copy

Within the Grid Editor, you may select *Tools > Grid Size Copy* or push down the ⬚ button on the toolbar to turn on the *Copy Grid Size* function. If this button is depressed, the column and row width of the current cell will be copied to all cells passed by the grid cursor.

3.5.18. Grid Split Copy

Within the Grid Editor, you may select *Tools > Grid Split Copy* or push down the ⬚ button on the toolbar to turn on the *Copy Grid Split Factor* function. If this button is depressed, the column and row split factors of the current cell will be copied to all cells passed by the grid cursor

3.5.19. Tools > Data Menu

Within the Data Editor, you may use this menu to manipulate cell-by-cell data of the current layer and/or the entire model. A menu item is dimmed, if it is not supported.

1. **Matrix:** Select this menu item to open the Matrix dialog box that displays cell values in a table. This function is available only when editing IBOUND, ICBUND, Layer Top/Bottom elevations, aquifer parameters, concentration values, and certain flow packages with matrix-based input data, such as Evapotranspiration or Recharge packages. The features of the Matrix dialog box are as follows.

   - **Table**: The table displays cell values of the selected parameter. The columns and rows of the table correspond to the model columns and rows. You may edit the value of a cell by clicking on the cell and then typing in the desired value. You may edit the values of a group of cells by selecting those cells with the mouse, and then typing in the desired value.

- **Parameter**: The cell values of the selected parameter are displayed in the table.

- **Column Width:** This defines the display width of the columns of the table.

- **Statistics:** This line contains the statistics of the displayed values.

2. **Reset:** Select this menu item to open the Reset dialog box, which is used to assign uniform cell values to the current model layer or to the entire model.

   The options *Apply to the entire model* and *Apply to the current layer* are available when editing IBOUND, ICBUND, layer top/bottom elevations, aquifer parameters, or concentration values.

   - **Apply to the entire model**: If this option is selected, the specified value(s) in the Reset Matrix dialog box will be applied to all cells of the entire model.

   - **Apply to the current layer:** If this option is selected, the specified value(s) in the Reset Matrix dialog box will be applied to all cells of the current model layer.

3. **Modify:** Open the Modify Data dialog box (Figure 32). This allows you to modify or display cell values of the current layer.

   - **Parameter:** The modification operation applies to the selected parameter.

   - **Filters:** The modification operation applies to the cells located within the *Target Area* and with the selected parameter values lying within the given *Search Range*. Target Area includes Current Layer, Views (Section 2.1) and Polygons (Section 3.3.2.3).

Figure 32. The Modify Data dialog box

   - **Value:** The user-specified value that is used to modify the cell values.

   - **Manipulation:** The final cell values are obtained by cell-by-cell calculation according to the selected manipulation rule as follows.

     o **None (display only):** No modification takes place.
     o **Replace:** Final cell value = the user-specified value.
     o **Add:** Final cell value = current cell value + the user-specified value.
     o **Subtract**: Final cell value = current cell value - the user-specified value.
     o **Multiply:** Final cell value = current cell value × the user-specified value.
     o **Divide**: For a non-zero user-specified value, final cell value = current cell value / the user-specified value. If the user-specified value equals to zero, the cell value remains unchanged.
     o **Minimum:** Final cell value = minimum of the user-specified value and current cell value.

o **Maximum:** Final cell value = maximum of the user-specified value and current cell value.

o **Average:** Final cell value = average of the user-specified value and current cell value.

4. **Import:** Open the Import Data dialog box (Figure 33) that allows you to import cell values from several types of files.

- **File:** Click the ⬚ button to select a file to be imported. After selecting a file, PM will attempt to determine its file type. If a supported file type is determined, the *File Type* dropdown box (see below) will be updated accordingly.

- **File Type:** The following file types are supported when editing IBOUND, ICBUND, and Layer Top/Bottom elevations, aquifer parameters, concentration values, and certain flow packages with matrix-based input data, such as Evapotranspiration or Recharge package. Refer to Section 5.1 for the formats of these file types.

o **2D Matrix**
o **2D Modflow Array**
o **3D Modflow Array**
o **SURFER ASCII GRD File**[22]
o **Comma-Separated Values File**[23]
o **ASCII Raster**[24]
o **Shapefile** [25] as defined by (ESRI, 1998).

For packages with list-based input data[26], the following file types are supported. If the file types 2D Matrix or 2D Modflow Array are used, the imported data only apply to existing instances of package-specific features, such as Hydraulic Conductance of rivers or drains.
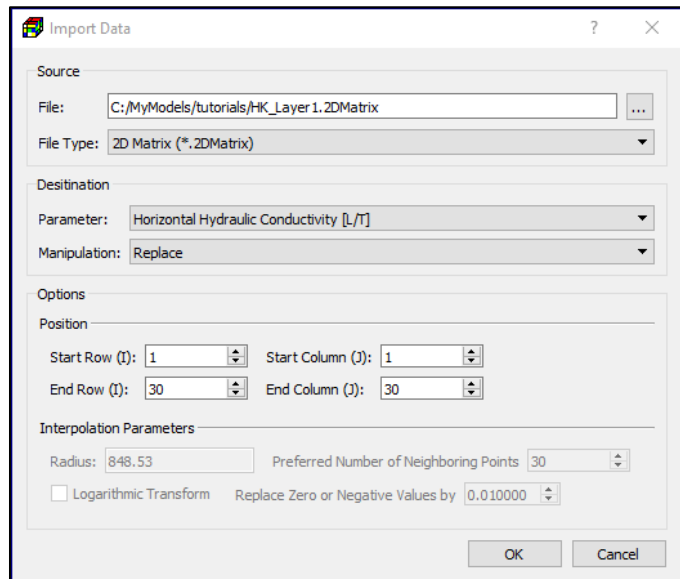
Figure 33. The Import Data dialog box

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[22] Only models with uniform column width and row width are supported. The GRD files must be saved in the Surfer ASCII GRD file format.

[23] Input values are interpolated to the model cells using the Interpolation Parameters.

[24] A projection file[3] is required for geo-referencing of an ASCII Raster file.

[25] Only shapefile with polygon or polyline features are supported. Before importing a selected shapefile, you need to select a column field from the shapefile attribute table. The selected attribute of a polygon will be imported to a cell, if its center lies within the polygon. The selected attribute of polyline vertices will be used for interpolation to cells.

[26] These packages use list-based input data: CHD, DRN, DRT1, FHB1, GHB, HFB6, MNW1, RES, RIV, STR, SFR2, and WEL.

- o **Package-specific format**[27]
- o **2D Matrix**
- o **2D Modflow Array**

- **Parameter:** The import operation will be applied to the selected parameter.

- **Manipulation:** The final imported cell values are obtained by cell-by-cell calculation according to the selected manipulation rule as follows.

  - o **Replace**: Final cell value = imported cell value.
  - o **Add**: Final cell value = current cell value + imported cell value.
  - o **Subtract**: Final cell value = current cell value - imported cell value.
  - o **Multiply**: Final cell value = current cell value × imported cell value.
  - o **Divide**: For a non-zero imported cell value, final cell value = current cell value / imported cell value. For an imported cell value that equals to zero, the cell value remains unchanged.
  - o **Minimum**: Final cell value = minimum of the current cell value and imported cell value.
  - o **Maximum**: Final cell value = maximum of the current cell value and imported cell value.
  - o **Average:** Final cell value = average of the current cell value and imported cell value.

- **Position**: Define the subgrid (by default, the entire grid) where the data will be imported to.

  - o If a 2D Matrix, 2D Modflow Array, 3D Modflow Array, or SURFER ASCII GRD file is used, the matrix values will be imported to the defined subgrid. The value located at [i, j] of the imported matrix will be imported to the cell located at [i + StartRow - 1, j + StartColumn - 1], if the cell location is valid.
  - o If a Comma-Separated Values File or an ASCII Raster is use, the input values will be interpolated to the cells of the subgrid. The resulting matrix with the interpolated values will then be imported in the same way as described above.

- **Interpolation Parameters:** These parameters are used to interpolate the input values from the Comma-Separated Values file, the ASCII Raster file, or the Shapefile with polyline features to the model grid. The interpolation process is based on a weighted method. In this method, the grid value C_{ij} at the cell [j, i] is the weighted average of surrounding data values, i.e.,

$$C_{ij} = \sum_{k=1}^{n} C_k W_k(r) / \sum_{k=1}^{n} W_k(r),$$

where C_k is the measured value at the kth measuring point, n the number of surrounding data values, $W_k(r)$ is the weighting function, and r the distance from the

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[27] Files in a package-specific format are created by using Tools > Data > Export.

grid point to the measuring point. The key component of a weighted method is the weighting function. A survey of weighting functions is presented by (Goodin, et al., 1979). In PM, the weighting function developed by Shepard (1968) is used, which improves the pure inverse distance weighting method by adding functions to dynamically determine (1) the radius of influence based on data density and distribution, and (2) the weighting factors based on distance between model cells and data points in the interpolation algorithm.

- o **Radius** and **Preferred Number of Neighboring Points** (PNP)**:** These values determine the neighboring data points that should be used to estimate the value at that cell with the following rules:

  - The number of points within the Radius (NPR) of the grid cell is determined by PM with a fast search algorithm (Mount, et al., 2010).
  - The number of neighboring points (NP) used by the Shepard's method to estimate the value at the grid cell is determined as follows:
  $NP = MinNP \quad if\ NPR < MinNP,$
  $NP = NPR \quad\quad if\ MinNP < NPR < MaxNP, and$
  $NP = MaxNP \quad if\ NPR > MaxNP,$
  where $MinNP = PNP \times 2/3$ and $MaxNP = PNP \times 4/3$
  - The radius used by the Shepard's method is the radius that encompasses those NP points next to the grid cell.

- o **Logarithmic Transform:** Check this box to log-transform the input values prior to performing interpolation. This is typically necessary if the input data is positively skewed, such as concentration measurements. Without log-transformation, the estimates based on positively skewed data sets could be significantly higher (over-estimation) because of the impact of high values.
- o **Replace Zero or Negative Values by:** Prior to log-transform, the input values that are smaller than or equal to zero are replaced by the value defined here.

5. **Copy:** Open the Copy Data dialog box (Figure 34) that allows you to copy cell values from the selected source to destination.
   - **Source:** This group defines the source data that may be copied to destination.
     - o **Parameter:** This dropdown box contains a list of static parameters (e.g., layer top elevation, layer bottom elevation, IBOUND, ICBUND, HK, VK, etc.).
     - o **Layer:** This dropdown box contains a list of layer numbers and an entry called *Entire Model*.

       - If a layer number is selected and the *Layer* dropdown box of the *Destination* group is set to *Current Layer,* the data of the selected layer will be copied to the current layer of the destination parameter.

- If a layer number is selected and the *Layer* dropdown box of the *Destination* group is set to *Entire Model,* the data of the selected layer will be copied to every layer of the destination parameter.
- If *Entire Model* is selected, the *Layer* dropdown box of the *Destination* group will also be set to *Entire Model,* and the data of the entire model will be copied to the entire model of the destination parameter
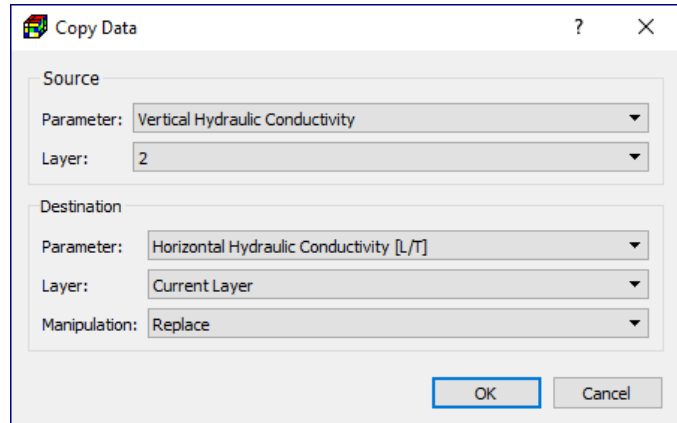
Figure 34. The Copy Data dialog box

- **Destination:** *Parameter* and *Layer* define the destination where the source data will be copied to.
  - **Parameter:** the source data will be copied to the selected parameter. For packages with list-based input data[26], the data only apply to existing instances of package-specific features, such as wells or drains.
  - **Layer:** this dropdown box contains *Current Layer* and *Entire Model*. See Layer in the Source group above for details.
  - **Manipulation:** The final cell values that are copied to the destination are obtained by cell-by-cell calculation according to the selected manipulation rule as follows, where *current value* is the current cell value of the destination parameter and source *value* is the cell value of the source data.

    - **Replace**: Final cell value = source value.
    - **Add**: Final cell value = current value + source value.
    - **Subtract**: Final cell value = current value - source value.
    - **Multiply**: Final cell value = current value × source value.
    - **Divide**: For a non-zero source value, final cell value = current value / source value. For a source value that equals to zero, the cell value remains unchanged.
    - **Minimum**: Final cell value = minimum of the current value and source value.
    - **Maximum**: Final cell value = maximum of the current value and source value.
    - **Average:** Final cell value = average of the current value and source value.

6. **Export:** Open the Export Data dialog box (Figure 35).
   - **File:** Click the ⬚ button to select a file to be exported.
   - **Parameter:** The data of the selected parameter will be exported.

- **Save As:** The exported file type. The following file types (refer to Section 5.1 for their formats) are supported when editing IBOUND, ICBUND, and Layer Top/Bottom elevations, aquifer parameters, concentration values, and certain flow packages with matrix-based input data, such as Evapotranspiration or Recharge package. For packages with list-based input data[26], package-specific formats are supported instead.
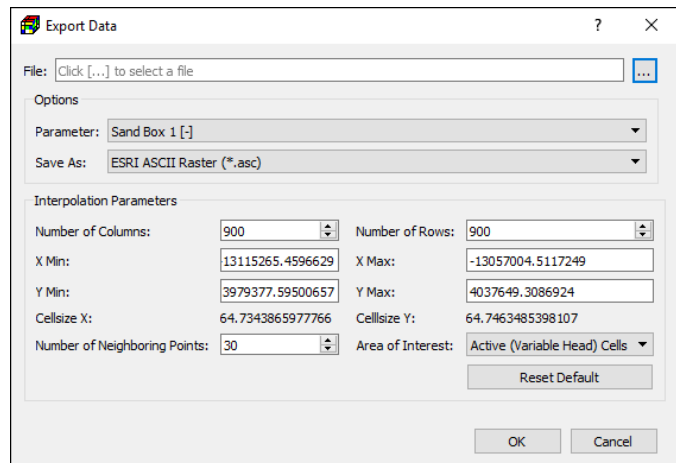
Figure 35. The Export Data dialog box

- o **2D Matrix**[28]
- o **2D Weight Matrix**[28]
- o **2D Modflow Array**
- o **3D Modflow Array**
- o **SURFER ASCII GRD File**[22]
- o **Comma-Separated Values File**[29]
- o **ASCII Raster**[30]

- **Interpolation Parameters:** This group is enabled only if the selected file type is ASCII Raster. When exporting to this format, the cell-by-cell values of the selected parameter are interpolated to a raster defined by the parameters of this group. The cell values equal to Nodata_Value (-1E20) are excluded from the interpolation. The interpolation is based on the Shepard's method (see above).

  - o **Number of Columns** and **Number of Rows**: The exported raster will have the defined numbers of columns and rows.
  - o **X Min**, **X Max, Y Min,** and **Y Max:** These are respectively the minimum and maximum X and Y coordinates (expressed in the Mercator coordinate system) of the raster. The default values cover the entire model grid.
  - o **Cellsize X** and **Cellsize Y**: These are respectively the column and row widths of the raster. These values are calculated based on the input values given above.

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[28] 2D Matrix and 2D Weight Matrix share the same format. In the latter, the cell values are divided by the sum of cell values in the layer before exporting. If the sum of cell values is zero, it is replaced by 1.

[29] The coordinates of the exported files are expressed in [longitude, latitude], where longitude and latitude are expressed in WGS84.

[30] The Mercator coordinates will be used in the exported raster file. A projection file[3] will be created along with the raster file.

- o **Number of neighboring points:** This defines the number of neighboring data points that should be used to estimate the value at a raster cell.
- o **Exclude Inactive (no-flow) Cells:** If this box is checked, values of inactive cells are not used for the interpolation.
- o **Area of Interest:** Cell-by-cell values are interpolated to the raster points within the selected area of interest and Nodata_Value (-1E20) is assigned to all other raster points. The results of the options "All" and "Model Bounding Box" are the same if the model grid is not rotated (or one of the model grid axes is parallel to a meridian).
- o **Reset Default:** Click this button to reset the values of numbers of columns and rows, as well as X Min, X Max, Y Min, and Y Max to their default settings.

3.5.20. Tools > Package Menu

1. **Replace Package:** When editing one of the following flow packages of MODFLOW, you may replace the data of a package by importing an input file that is stored in the format as described in the user guide of MODFLOW (Harbaugh, 2005) or the package-specific document. Select this menu item and select an input file of the package from the Open File dialog box. Make sure that the correct file format, e.g., *MODFLOW-2005 Free Format* or *MODFLOW-2005 Fixed Format*, is selected in the Open File dialog box. Choose *MODFLOW-2005 Free Format,* if the input file was created by PM.

- Drain Package
- Drain with Return Flow Package
- Evapotranspiration Package
- Evapotranspiration Segments Package
- Flow and Head Boundary Package
- General-Head Boundary Package
- Horizontal-Flow Barrier Package
- Interbed-Storage Package
- Lake Package
- Multi-Node Well (MNW1) Package
- Recharge Package
- Reservoir Package
- River Package
- Stream (STR) Package
- Streamflow-Routing (SFR2) Package[16]
- Subsidence and Aquifer Compaction Package
- Seawater Intrusion 2 (SWI2) Package
- Time Variant Specified Head Package
- Unsaturated-Flow (UZF1) Package
- Well Package

2. **Append Package:** This menu item works in the same way as *Replace Package* above, except that the existing data of a package will <u>not</u> be cleared prior to importing the data from an input file.

3. **Append Wells:** When editing the Well package, you may import wells from a Well file that stores coordinates and screen intervals of wells, as well as their pumping/injection rates per stress period, and optionally the concentration of the injection fluid. Refer to Section 5.1.16 for the format of the Well file. When importing a well file, pumping/Injection rate of a well is prorated to the vertical column of cells where the well is located based on the following equation. The imported data will be appended to the existing data.

$$Q_i = \frac{Q_w \times HK_i \times L_i \times F_i}{\sum_{i=1}^{NLAY}(HK_i \times L_i \times F_i)}$$

where

i is the layer number,

HK_i is the hydraulic conductivity of the cell in the ith layer,

L_i is the total length of saturated well screen(s) within the cell in the ith layer; the values of starting hydraulic head, layer geometry, and screen intervals are used to calculate the saturated well-screen length,

F_i = 1 if the cell in the ith layer is a variable head (active) cell; and F_i = 0 if no-flow (inactive),

Q_w is the pumping/injection rate of the well,

Q_i is the pumping/injection rate that is assigned to the cell in the ith layer.

4. **Remove Wells:** When editing the Well package, you may remove wells from all stress periods with pumping rates lie between two user-specified flow rate values.

5. **Clear Package**: Clear all data of the package that is being edited.

3.6. Discretization Menu

3.6.1. Time

The menu item opens the Time dialog box (Figure 36) that defines the temporal discretization scheme of the model.

1. **Time Unit**: This dropdown box defines the time unit of the model data and stress period length.

2. **Auto Update Period Length**: If this box is checked, the stress period length will be updated whenever the time unit is changed. The values of all other model parameters are not affected.

3. **Table:** MODFLOW divides the total time length of a simulation into stress periods, which are, in turn, divided into time steps. The table displays the temporal discretization data.

- **Period** is the stress period number.

- **Steady State**[31]: Check the box, if a period is steady state; uncheck the box if transient.

- **PERLEN** is the length of a stress period, expressed in the unit selected by the Time Unit dropdown box. The sum of all PERLEN values is defined as the Simulation Length of the flow simulation. In a MODFLOW simulation, Simulation Time starts at 0 and increases throughout the course of the simulation.

- **NSTP** is the number of time steps within a stress period.

- **TSMULT** is the time step multiplier, which is the ratio of the length of each time step to that of the preceding time step. The length of the first time step, $\Delta t1$, is related to PERLEN, NSTP, and TSMULT by the relation:

$$\Delta t1 = PERLEN \cdot \left(\frac{TSMULT-1}{TSMULT^{NSTP}-1} \right) \tag{3}$$

- **DT0** is the initial transport step length within each time step of the flow solution. If DT0 is specified as zero, the actual value of DT0 is calculated based on the Courant number specified in the Advection package. The subsequent transport step size depends on the value of TTSMULT and the solution scheme for the advection term.

Period	Steady State	PERLEN	NSTP	TSMULT	DT0	MXSTRN	TTSMULT	TTSMAX
1	☐	30.5	1	1.2	0.5	500	1.25	0
2	☐	30.5	1	1.2	0.5	500	1.25	0
3	☐	30.5	1	1.2	0.5	500	1.25	0
4	☐	30.5	1	1.2	0.5	500	1.25	0
5	☐	30.5	1	1.2	0.5	500	1.25	0
6	☐	30.5	1	1.2	0.5	500	1.25	0
7	☐	30.5	1	1.2	0.5	500	1.25	0
8	☐	30.5	1	1.2	0.5	500	1.25	0
9	☐	30.5	1	1.2	0.5	500	1.25	0
10	☐	30.5	1	1.2	0.5	500	1.25	0
11	☐	30.5	1	1.2	0.5	500	1.25	0
12	☐	30.5	1	1.2	0.5	500	1.25	0
13	☐	30.5	1	1.2	0.5	500	1.25	0
14	☐	30.5	1	1.2	0.5	500	1.25	0
15	☐	30.5	1	1.2	0.5	500	1.25	0

Time Unit: Day ☐ Auto Update Period Length

Click a column header to set a default value to all stress periods. Hover over a column header to display its description.

Add Delete More Actions▼ OK Cancel

Figure 36. The Time dialog box

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[31] If the Interbed Storage (IBS) Package is used, only the first stress period may be steady state.

- **MXSTRN** is the maximum number of transport steps allowed within a time-step of the flow solution. If the number of transport steps within a flow time step exceeds MXSTRN, the simulation is terminated.

- **TTSMULT** is the multiplier for successive transport steps within a flow time-step if the solution option for the advection term is the standard finite-difference method. A value between 1.0 and 2.0 is generally adequate. For the particle-tracking-based solution options and the third order TVD scheme, TTSMULT does not apply.

- **TTSMAX** is the maximum transport step size allowed when transport step size multiplier TTSMULT > 1.0. The limit is lifted by setting TTSMAX = 0.

4. **Add:** Click this button to add a row (i.e., a stress period) to the table.

5. **Delete:** Click this button to delete the selected row from the table.

6. ***More Actions > Save:*** Save the contents of the table to a *Temporal Discretization* file. See Section 0.⍰ for the file format.

7. ***More Actions > Load:*** Populate the table with the contents of a Temporal Discretization file that was previous created with the *More Actions > Save.*

8. **OK:** Accept and save the changes.

3.6.2. Grid

Select this menu item to edit the model grid. See the Grid Editor (Section 3.3.1) for details.

3.6.3. Layer Property

The menu item opens the Layer Property dialog box (Figure 37). You can specify the properties of individual layers in the table.

Layer	Layer Type	Method	Color	HANI	VK/VANI	T	VCONT	S	IBS	TRPT	TRPV
1	Convertible	Harmonic mean		1	VK	Calculated	Calculated	Calculated	☐	0.100	0.010
2	Confined	Harmonic mean		1	VK	Calculated	Calculated	Calculated	☐	0.100	0.010
3	Confined	Harmonic mean		1	VK	Calculated	Calculated	Calculated	☐	0.100	0.010
4	Confined	Harmonic mean		1	VK	Calculated	Calculated	Calculated	☐	0.100	0.010
5	Confined	Harmonic mean		1	VK	Calculated	Calculated	Calculated	☐	0.100	0.010

Figure 37. The Layer Property dialog box

1. **Layer** is the layer number. Model layers are numbered from the top down.
2. **Layer Type** affects the numerical formulation of the groundwater flow equation. The available options and required parameters depend on the select internal flow package. Note that S, S, and Sy are used only in transient flow simulations.

   - **BCF Package** supports the following layer types:

     o **Confined**:
       - Required input parameters: T and S
       - Interblock conductance is calculated based on input values of T, and therefore remains unchanged for the entire simulation.

     o **Unconfined**: The option is valid only for layer 1.
       - Required input parameters: HK and Sy.
       - Interblock conductance is calculated based on HK and saturated thickness that may vary during a flow simulation.

     o **Limited Convertible** between confined and unconfined.
       - Required input parameters: T, S, and Sy.
       - Interblock conductance is calculated based on input values of T, and therefore remains constant for the entire simulation regardless of the saturated thickness.
       - If the layer is fully saturated, the storage is calculated based on S; Otherwise Sy and saturated thickness are used.
       - Vertical flow from above is limited if the layer desaturates.

     o **Full Convertible** between confined and unconfined.
       - Required input parameters: HK, S, and Sy.
       - If the layer is not fully saturated, the storage is calculated based on Sy and the saturated thickness; and the interblock conductance is calculated based on HK and the saturated thickness.
       - If the layer is fully saturated, the storage is calculated based on S; and the interblock conductance is calculated based on HK and the layer thickness.
       - Vertical flow from above is limited if the layer desaturates.

   - **LPF** or **UPW Package** supports the following layer types:

     o **Confined**:
       - Required input parameters: HK, Ss, and VK or VANI.
       - Interblock conductance is calculated based on HK and layer thickness, and therefore remains constant for the entire simulation.
       - The storage is calculated based on Ss and layer thickness.
       - VK or VANI is used for calculating vertical conductance between layers.

o **Convertible** between confined and unconfined.

- Required input parameters: HK, Ss, Sy, and VK or VANI.
- If the layer is not fully saturated, the storage is calculated based on Sy and the saturated thickness; and the interblock conductance is calculated based on HK and the saturated thickness.
- If the layer is fully saturated, the storage is calculated based on Ss and the layer thickness; and the interblock conductance is calculated based on HK and the layer thickness.
- VK or VANI is used for calculating vertical conductance between layers.

3. **Method** defines the method of calculating interblock transmissivity.

4. **Color** defines the color that is used to draw observation points and pathlines when they reside within the respective layer.

5. **HANI** defines the ratio of the HK along columns to HK along rows.

- **BCF package:**

   o The absolute values of HANI are assigned to the TRPY array (i.e., an array containing a horizontal anisotropic factor for each layer) in the BCF's input file.

- **LPF or UPW package:**

   o If HANI > 0, the specified HANI value is assigned to all cells in the layer.
   o If HANI < 0, the values specified in *Parameters > Horizontal Anisotropy* are used for the layer.

6. **VK/VANI** determines whether vertical hydraulic conductivity or vertical anisotropy is used for a layer.

- **BCF package:**

   o This column is dimmed as input of VANI is not supported by BCF.

- **LPF or UPW package:**

   o **VK** indicates that the values specified in *Parameters > Vertical Hydraulic Conductivity* are used for the layer.
   o **VANI** indicates that values specified in *Parameters > Vertical Anisotropy* (i.e., ratio of horizontal to vertical hydraulic conductivity) are used for the layer.

7. **T** determines how transmissivity values are defined.

- **BCF package** requires transmissivity values for layers of the types **Confined** or **Limited Convertible**. To facilitate the data input, two options are available

   o **User-Specified:** The values specified *in Parameters > Transmissivity* are used for the layer.

- o **Calculated:** The product of the layer thickness (i.e., layer top elevation – bottom elevation) and the values specified in *Parameter > Horizontal Hydraulic Conductivity* (i.e., HK) are used for the layer.

- **LPF or UPW package:**
  - o This column is dimmed as input of T is not supported.

8. **VCONT** determines how vertical leakance values are defined.
- **BCF package** requires the input of vertical leakance (VCONT [T^{-1}]) values to all layers, except for the bottom layer. This option determines whether user-specified or calculated VCONT values should be used. For the latter, VCONT is calculated based on VK and layer thickness.
  - o **User-Specified:** The values specified in *Parameters > Vertical Leakance* are used in the simulation. In the Data Editor, VCONT between the layers i and i+1 is entered to the ith layer.
  - o **Calculated:** VCONT is calculated with Equation (4). The calculated values are used in the simulation.

$$VCONT = \frac{2}{\frac{m_k}{(VK)_{k,i,j}} + \frac{m_{k+1}}{(VK)_{k+1,i,j}}} \quad (4)$$

  where $(VK)_{k,i,j}$ and $(VK)_{k+1,i,j}$ are the vertical hydraulic conductivity values of the layer k and layer k+1, respectively. m_k and m_{k+1} are the thickness of the layer k and k + 1, respectively.

- **LPF or UPW package:**
  - o This column is deactivated as direct input of VCONT is not supported. These packages calculate VCONT internally base on Equation (4).

9. **S** determines how values of confined storage coefficient are defined in a transient flow simulation. When a layer is unconfined, the storage term is defined by specific yield [-] and the setting of **S** does not apply.
- **BCF package:** For a confined layer, these storage terms are given by the confined storage coefficient (=specific storage [L^{-1}] × layer thickness [L]).
  - o **User-Specified:** The values specified in *Parameters > Storage Coefficient* are used in the simulation.
  - o **Calculated:** The product of the layer thickness (i.e., layer top elevation – bottom elevation) and the values specified in *Parameter > Specific Storage* (i.e., Ss) are used for the layer.

- **LPF or UPW package:**
  - o This column is deactivated as LPF and UPW packages always requires the input of specific storage (Ss) values for confined layers.

10. **IBS:** When the Interbed Storage package is activated, this option turns on/off the calculation of storage changes and compaction for specific layers.

11. **TRPT** is the ratio of the horizontal transverse dispersivity to the longitudinal dispersivity. TRPT is used by MT3D and SEAWAT.

12. **TRPV** is the ratio of the vertical transverse dispersivity to the longitudinal dispersivity. TRPV is used by MT3D and SEAWAT.

3.6.4. Layer Top Elevation and Layer Bottom Elevation

Select *Discretization > Layer Top Elevation* or *Discretization > Layer Bottom Elevation* to define, respectively, the top or bottom elevations of the model cells with the Data Editor.

3.6.5. IBOUND (Flow)

MODFLOW requires an IBOUND array, which contains a value for each model cell. A positive value in the IBOUND array defines a variable-head (i.e., active) cell where the hydraulic head is computed, a negative value defines a constant head cell and the value 0 defines a no-flow cell (i.e., inactive) cell. It is suggested to use 1 for variable-head cells, 0 for no-flow cells and -1 for constant head cells. Flux boundaries may be simulated by assigning appropriate fluxes with the Flow and Head Boundary or the Well package.

For constant head cells, the hydraulic head is hold at the starting value throughout the simulation. The starting hydraulic head is specified in *Parameters > Starting and Prescribed Hydraulic Heads*. A constant head boundary exists when an aquifer is in direct hydraulic contact with a river, a lake, or a reservoir in which the water (groundwater) level is known to be constant. It is important to know that constant head boundaries can provide inexhaustible supply or sink of water. Care must be taken when using constant head boundaries, as a groundwater system may get or lose unrealistically much water as necessary from or to such a boundary. It is recommended to avoid using this boundary condition on the upstream side of the groundwater flow direction. Consider using the General-Head Boundary or the Time-Variant Specified-Head packages, if the hydraulic head at the constant head boundary varies with time. Head-dependent boundary conditions may be simulated by means of the general head boundary, river, stream, reservoir or drain package.

3.6.6. ICBUND (Transport)

The transport models MT3D and SEAWAT require an ICBUND array, which contains a value for each model cell. A positive value in the ICBUND array defines an active concentration cell (the concentration varies with time and is calculated), a negative value defines a constant-concentration cell (the concentration is constant) and the value 0 defines an inactive concentration cell (no transport simulation takes place at such cells). It is recommended to use the value 1 for an active concentration cell, -1 for a constant-concentration cell, and 0 for an inactive concentration cell. Note that the ICBUND array applies to all species. Other types of

boundary conditions are implemented by assigning concentrations to inflows or assigning a mass-loading rate to cells. For details, see Section 3.8.3.3.4.

No-flow or dry cells are automatically converted to inactive concentration cells. Variable-head cells may be treated as inactive concentration cells to minimize the area needed for transport simulation, if the solute transport is insignificant near those cells. For constant-concentration cells, the initial concentration remains the same at the cell throughout the simulation. A constant head cell may or may not be a constant-concentration cell. The initial concentration is specified in *Models > Transport (MT3D/SEAWAT) > Initial Concentration*.

3.7. Parameters Menu

3.7.1. Starting Hydraulic Head

MODFLOW requires a starting hydraulic head value (starting head [L]) for each model cell at the beginning of a flow simulation. Starting heads at constant head cells are used as prescribed head values and remain constant throughout the flow simulation.

For steady-state flow simulations, the starting heads are used as initial values for the iterative equation solvers and should be set as close as possible to the final head solution. For an unconfined or a convertible layer, the starting head of a constant head cell must be higher than the elevation of the cell bottom. Otherwise, MODFLOW will write the message *CONSTANT-HEAD CELL WENT DRY – SIMULATION ABORTED* to its run listing file and then abort the simulation.

In a transient flow simulation, the starting heads provide a reference elevation for the solution. It is a standard practice to use heads generated by a steady-state model as the initial conditions for a transient model, see Section 7.4 of (Anderson, et al., 2015) for more details.

3.7.2. Horizontal Hydraulic Conductivity (HK) and Transmissivity (T)

HK [L/T] is the horizontal hydraulic conductivity along model rows. T [L^2/T] is the product of HK and layer thickness. Typical values and ranges of HK for diverse types of soils are given in many groundwater textbooks, for example (Freeze, et al., 1979), (Spitz, et al., 1996) and (Fetter, 1994).

If the BCF package is selected as the internal flow package, HK is required for *unconfined* and *full convertible* layers and T is required for *confined* or *limited convertible* layers. You have the option to specify T directly by selecting *Parameters > Transmissivity* or specify HK by selecting *Parameters > Horizontal Hydraulic Conductivity* and let PM calculate T by using the layer thickness and HK. See Section 3.6.3 for details.

If the LPF or UPW package is selected as the internal flow package, HK is required for all layer types and direct input of T is not possible.

3.7.3. Horizontal Anisotropy (HANI)

HANI [-] is the ratio of horizontal hydraulic conductivity along columns to horizontal hydraulic conductivity along rows.

If the BCF package is selected as the internal flow package, this menu item is deactivated as the BCF only supports the input of layer-by-later HANI values and does not support the cell-by-cell HANI values. Use the Layer Property dialog box (Section 3.6.3) to input the layer-by-layer HANI values.

If the LPF or UPW package is selected as the internal flow package, you may use this menu item to enter the cell-by-cell HANI values. The entered values may or may not be used in a simulation, depending on the settings of the HANI column in the Layer Property dialog box. See Section 3.6.3 for details.

3.7.4. Vertical Hydraulic Conductivity (VK) and Vertical Leakance (VCONT)

 The vertical leakance between two vertically adjacent cells is calculated based on Equation (4). The VCONT value is multiplied by cell area to obtain vertical conductance, which is used for formulating the vertical flow term by MODFLOW.

If the BCF package is selected as the internal flow package, an array of VCONT values is required for each layer, except for the bottom layer. You have the option to specify VCONT directly by selecting *Parameters > Vertical Leakance or* specify VK by selecting *Parameters > Vertical Hydraulic Conductivity* and let PM calculate VCONT. See the setting of VCONT in Section 3.6.3 for details.

If the LPF or UPW package is selected as the internal flow package, VCONT is calculated for all layer types by LPF or UPW internally. The calculation is based on VK or Vertical Anisotropy. A direct input of VCONT is not possible.

3.7.5. Vertical Anisotropy (VANI)

VANI is the ratio of HK to VK.

If the BCF package is selected as the internal flow package, this menu item is deactivated as the input of VANI is not supported.

If the LPF or UPW package is selected as the internal flow package, you have the option to enter VK directly by selecting *Parameters > Vertical Hydraulic Conductivity* or enter VANI and let PM determine VK (= HK/VANI).

3.7.6. Specific Storage (Ss) and Storage Coefficient (S)

For a steady state simulation, these menu items are not used and are deactivated. S is required by MODFLOW for confined or convertible layers.

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

In a confined layer, the storage term is given by the *storativity* or *storage coefficient* [-] (= specific storage [L^{-1}] × layer thickness [L]). The storativity is sometimes referred to as *confined storage coefficient.*

If the BCF package is selected as the internal flow package, you have the option to enter S directly by selecting *Parameters > Storage Coefficient,* or enter Ss by selecting *Parameters > Specific Storage* and let PM calculate S. See the setting of S in Section 3.6.3 for details.

If the LPF or UPW package is selected as the internal flow package, Ss is required. A direct input of S is not possible.

3.7.7. Specific Yield (Sy)

For a steady state simulation, this menu item is not used and is deactivated. Sy is required by MODFLOW for unconfined or convertible layers.

Specific yield [-] is defined as the volume of water that an unconfined aquifer releases from storage per unit surface area of aquifer per unit decline in the water table. *Specific yield* is a function of porosity (and is not necessarily equal to porosity), because a certain amount of water is held in the soil matrix and cannot be removed by gravity drainage. Refer to (Spitz, et al., 1996) for a summary of values of specific yield. Refer to (Bear, 1972), (Bear, 1979) or (Freeze, et al., 1979) for detailed explanation of storage terms and their definitions.

3.7.8. Effective Porosity (ne)

Effective porosity is used by MODPATH, MT3D and SEAWAT for calculating the average velocity of the flow through the porous medium.

If the total unit volume V of a soil matrix is divided into the volume of the solid portion V_s and the volume of voids V_v, the total porosity n is defined as n = V_v/V. Effective porosity (with the respect to flow through the medium) is always less than total porosity, sometimes (as in the case of clays) much less, because some of the pore spaces may be too small or too poorly connected so that part of the fluid is immobile or partially immobile. A summary of representative porosity values for different soil types can be found in (Zheng, et al., 1995) or (Domenico, et al., 1997).

3.7.9. Stop Zone

Stop Zone is used by MODPATH to define stopping locations for particles. The Stop Zone option of MODPATH is activated by specifying a positive Stop Zone value to MODPATH's settings window (Figure 133). Particles stop, when they enter cells with the specified Stop Zone value.

3.7.10. Retardation Factor (R)

Retardation factor is used by MODPATH as a scaling factor for the magnitude of the velocity.

The retardation factor is a function of the porosity, the density of the geologic material, and the sorption coefficient. A detailed discussion of the retardation factor can be found in (Domenico, et al., 1997). The effect of linear sorption on the apparent velocity of a reactive solute can be examined using the particle-tracking method in MODPATH by dividing the velocity components by a retardation factor. For nonreactive solutes that do not interact with the surrounding rock, the retardation factor is equal to 1 and the magnitude of the apparent solute velocity is equal to that of the groundwater velocity. For solutes affected by linear sorption, the retardation factor is greater than 1 and the magnitude of the apparent solute velocity is less than that of the groundwater velocity.

3.7.11. Bulk Density

The cell-by-cell bulk density data are used by the Reaction package of MT3D and SEAWAT for simulating sorption effects.

3.7.12. Static Sandboxes

A Static Sandbox is a place where you can store data for visualization purposes. The values specified in a Static Sandbox do not vary with time and will not be used in simulation.

3.7.13. Transient Sandboxes

A Transient Sandbox is a place where you can store time-dependent data for animation and visualization purposes. For a model with multiple stress periods, the user may assign various matrix values to (the end of the selected) stress periods. If a contour map is created with the data of transient sandbox, the contour map will transit between stress periods based on the linearly interpolated matrix values of those stress periods.

3.8. Models Menu

3.8.1. MODFLOW

3.8.1.1. Packages

To activate a package and edit its data, select the respective menu item. If the package is already activated, you will have the opportunity to edit its data or deactivate the package.

3.8.1.1.1. Drain (DRN)

The Drain (DRN) Package is used to simulate effects of features such as agricultural drains, which remove groundwater from aquifer at a rate proportional to the head difference between the aquifer and the drain.

A drain is implemented by dividing into drain segments so that each drain segment is completely contained in a single model cell. Multiple drain segments may be assigned to a model cell. For

each drain segment, the recharge rate from the drain to the model cell is always zero, and the discharge rate from the model cell to the drain is calculated by

$$Q_d = C_d \cdot (h - h_d) \qquad \text{if } h > h_d \qquad\qquad (5)$$

$$Q_d = 0 \qquad\qquad\qquad \text{if } h <= h_d \qquad\qquad (6)$$

where

Q_d [L^{3}T^{-1}] is the discharge rate from the cell to the drain segment,

h [L] is the calculated hydraulic head in the cell containing the drain segment,

h_d [L] is the elevation of the drain segment, and

C_d [L^{2}T^{-1}] is the conductance of the drain segment.

The required input parameters are listed below.

1. **Cell-by-cell input method:** Figure 38 shows the dialog box for specifying one or more drain segments to a model cell. For each segment, the following properties need to be assigned.
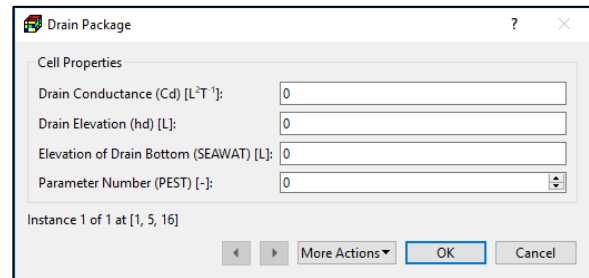
   Figure 38. The Drain Package dialog box for specifying cell properties

   - **Drain conductance (C_d) [L^{2}T^{-1}]** relates drain discharge rate to the head loss between the drain and the aquifer. The value of C_d depends on the material and characteristics of the drain and the immediate environment.

   - **Drain elevation (h_d) [L]** is the elevation of the drain segment.

   - **Parameter Number (PEST) [-]** is used to group cells, where the Cd value is to be estimated by PEST. See *To define an estimable parameter* in Section 3.8.4 for details.

   - **Elevation of drain bottom [L]** is used by SEAWAT to calculate reference head considering the density effect to accurately simulate the flow of variable-density ground water to a drain. For details, see DRNBELEV on the VDF tab of the Transport Settings dialog box (Figure 99).

2. **Polyline input method:** Figure 39 shows the dialog box that is used to specify polyline and vertex properties.

   - **Polyline Properties**
     o **Auto Layer Number:**
       - If this box is checked, the layer number of a drain segment alone the polyline is determined by comparing its drain elevation (HD) with the top/bottom elevations of the cells in the same vertical model column as that drain segment.

- if HD is higher than the top elevation of the highest cell, the drain segment is assign to the cell in layer 1.
- if HD is lower than the bottom elevation of the lowest cell, the drain segment is assigned to the cell in layer NLAY.
- If HD lies between top and bottom elevations of a cell, the drain segment is assigned to that cell.

  - If this box is not checked, the drain segments along the polyline are assigned to the layer where the polyline is located.
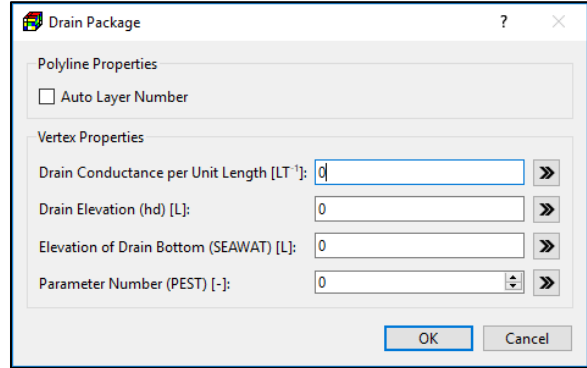
Figure 39. The Drain Package dialog box for specifying vertex properties

- **Vertex Properties:** The specified vertex data may be applied to model cells following the rules described in Section 3.3.2.2 and the rules below.

  o **Drain Conductance per Unit Length [LT^{-1}].** When applying the vertex data to model cells, the specified value is interpolated to the DRN cells along the polyline. For each of those cells, the interpolated cell value is multiplied with the length of the drain within the cell to obtain the drain conductance C_d.

$$C_d = C_{dl} \cdot L_c \qquad\qquad (7)$$

where

C_{dl} is the drain conductance per unit length at a given cell, and

L_c is the length of the drain within the cell.

  o **All other parameters:** Refer to the cell-by-cell input method above for the descriptions of these parameters.

3. **Polygon input method:** Figure 40 shows the dialog box that is used to specify polygon properties. The polygon data may be assigned to model cells following the rules described in Section 3.3.2.3 and the rules below.

- **Auto Layer Number:** See the description for the polyline input method above.

- **Drain Conductance per Unit Area [T^{-1}]:** When applying the polygon data
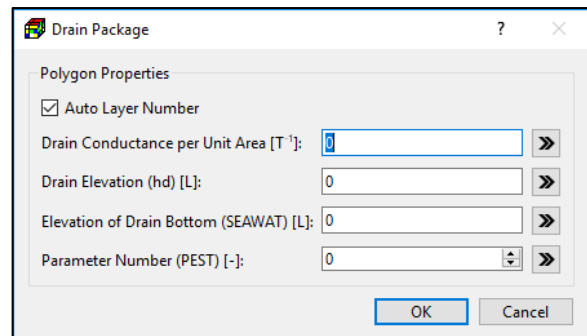
Figure 40. The Drain Package dialog box for specifying polygon properties

to model cells within the polygon, the specified value (C_{da}) is multiplied with the cell area to obtain the drain conductance C_d.

$$C_d = C_{da} \cdot Area_c \qquad\qquad (8)$$

where

C_{da} is the Drain Conductance per Unit Area,

$Area_c$ is the area of the cell.

  o **All other parameters:** Refer to the cell-by-cell input method above for the descriptions of these parameters.

3.8.1.1.2. Drain with Return Flow (DRT1)[32]

The Drain with Return Flow (DRT1) Package (Banta, 2000) can be used to simulate the return flow of water discharged from a drain back into the ground-water system. If the return-flow option of the DRT1 Package is enabled, for each cell designated as a drain-return cell, the user has the option of specifying a proportion of the water, simulated as leaving the ground-water system through the drain feature, to return to one other cell in the model.

The numerical formulation and most required parameters for the DRT1 Package are the same as those of the DRN Package. The parameters for the return flow function described below.

1. **All input methods:** The data entry dialog boxes of all input methods include a Simulation Settings group that contains the following options:

   - **Activate the Return-flow Option of the Drain Return Package:** Check this box to enable the return-flow feature of DRT.

   - **Include Concentration Data in the SSM Package of MT3D/SEAWAT:** If this box is checked, the values entered to **Concentration (MT3D/SEAWAT) [ML^{-3}]** are associated with the return flow. If this box is not checked,
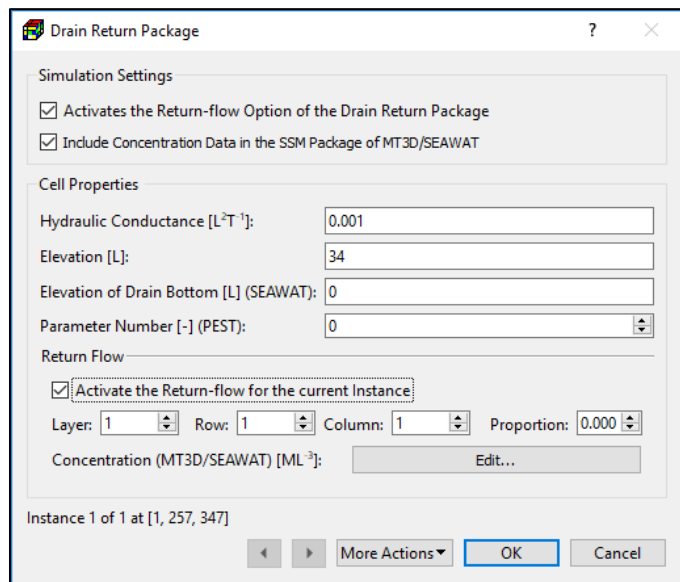
Figure 41. the Drain Return Package dialog box for specifying cell properties

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[32] It has been noticed that DRT1 and MNW1 packages may not be used as the same time with MT3DMS due to incompatibility between the LINK-MT3DMS (LMT) Package of MODFLOW and the Flow Model Interface (FMI) Package of MT3DMS.

the calculated concentration at the outflow cell will be associated with the return flow.

2. **Cell-by-cell input method:** Figure 41 shows the dialog box for specifying cell properties.

   - **Return Flow**

     o If the *Activate the Return-flow for the current Instance box* is checked, the current drain instance will be able to return a portion of water to the model cell at the [Layer, Row, Column]

     o **[Layer, Row, and Column]** defines the recipient cell where a portion of drain flow is returned to the groundwater system.

     o **Proportion**: The return-flow is equal to product of this value and the simulated drain flow.

     o **Concentration (MT3D/SEAWAT) [ML^{-3}]:** Click the **Edit** button to open the Concentration dialog box (Figure 42) that allows you to specify the return flow concentration of up to 100 species. You can either enter individual concentration values to the table directly or click the *Set Value* button to enter a uniform value for all species. The entered concentration values may be used by the SSM Package of MT3D or SEAWAT.

3. **Polyline input method:** Figure 43 shows the dialog box that is used to specify vertex/polyline properties.
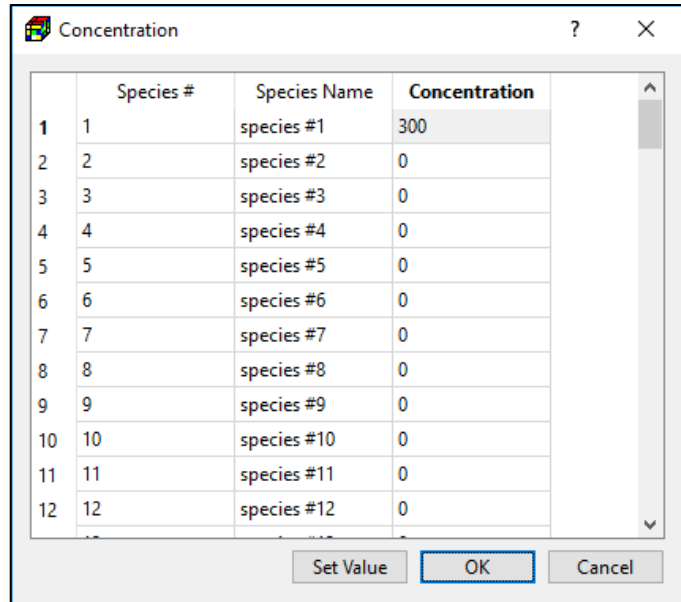
Figure 42. The Concentration dialog box
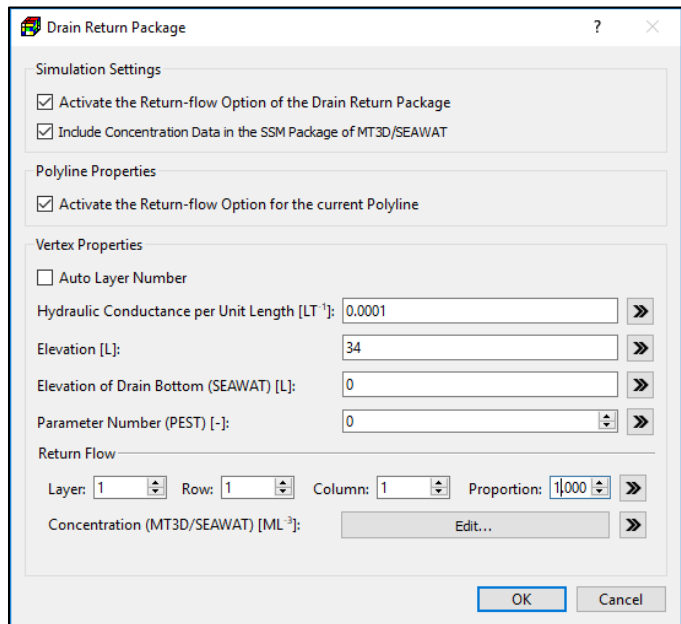
Figure 43. The Drain Return Package dialog box for specifying vertex/polyline properties

- **Polyline Properties:** If the *Activate the Return-Flow Option for the current Polyline* box is checked, the drain instances along the polyline will be able to return a portion of water to the model cells defined by [Layer, Row, Column] in the Return Flow below.

- **Vertex Properties:**

  o **Return Flow**

    – [**Layer, Row, and Column**]: defines the recipient cell(s) of return-flow.
    – **Proportion**: The return-flow is equal to product of this value and the simulated drain flow.
    – **Concentration (MT3D/SEAWAT) [ML^{-3}]:** Click the **Edit** button to open a Concentration dialog box (Figure 42) that allows you to specify the return flow concentration of up to 100 species to the current vertex.

4. **Polygon input method:** Figure 44 shows the dialog box that is used to specify polygon properties.

   - **Simulation Settings:** Check the *Activate the Return-flow Option of the Drain Return Package* box to enable the return-flow feature of DRT.

   - **Polygon Properties:** If the *Activate the Return-Flow Option for the current Polygon* box is checked, the drain instances within the polygon will be able to return a portion of water to the model cells defined by [Layer, Row, Column] in the Return Flow below.
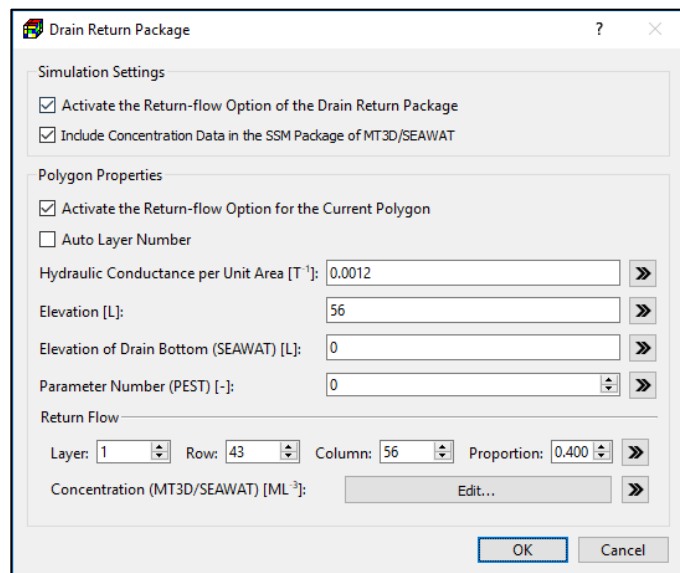
Figure 44. The Drain Return Package dialog box for specifying polygon properties

  o **Return Flow**

    – [**Layer, Row, and Column**]: defines the recipient cell of return-flow.
    – **Proportion**: The return-flow is equal to product of this value and the simulated drain flow.
    – **Concentration (MT3D/SEAWAT) [ML^{-3}]:** Click the **Edit** button to open a Concentration dialog box (Figure 42) that allows you to specify the return flow concentration of up to 100 species to the current polygon.

3.8.1.1.3. Evapotranspiration (EVT)

The Evapotranspiration (EVT) Package simulates the effects of plant transpiration and direct evaporation by removing water from the saturated groundwater regime. Evapotranspiration can be drawn from only one cell in each vertical column of model cells. The evapotranspiration rate is calculated for a cell in each vertical column of model cells by

$$R_{et} = EVTR \qquad\qquad\qquad\qquad \text{if } h > SURF \qquad\qquad\qquad (9)$$

$$R_{et} = EVTR \cdot \frac{h-(SURF-EXDP)}{EXDP} \qquad \text{if } (SURF\text{-}EXDP) \le h \le SURF \qquad (10)$$

$$R_{et} = 0 \qquad\qquad\qquad\qquad\qquad \text{if } h < SURF\text{-}EXDP \qquad\qquad (11)$$

where

R_{et} [LT^{-1}] is the rate of loss per unit surface area of water table due to evapotranspiration;

h [L] is the calculated hydraulic head in the cell from which the evapotranspiration occurs;

EVTR [LT^{-1}] is the maximum possible value of R_{et} or potential evapotranspiration rate;

$SURF$ [L] is the ET surface elevation;

$EXDP$ [L] is the cutoff or extinction depth.

The evapotranspiration flow rate Q_{et} [L^{3}T^{-1}] drawn from the model cell is

$$Q_{et} = R_{et} \times Area_c \qquad\qquad\qquad\qquad\qquad\qquad\qquad (12)$$

where $Area_c$ is the area of the model cell.

The required input parameters for all input methods are identical and listed below. Although these parameters are to be assigned to each vertical column of model cells, you may move between layers within the Data Editor to examine the grid configuration in each layer.

1. **All input methods:** Figure 45 shows the dialog box for specifying cell, vertex, or polygon properties.

   - **ET Option (NEVTOP) [-]**: Since Q_{et} is calculated for only one cell in each vertical column of model cells, three options are available for specifying the cell where Q_{et} is drawn from:

     o ET is calculated only for cells in the top grid layer.
     o ET is calculated for cells in the layers defined by IEVT (see below)
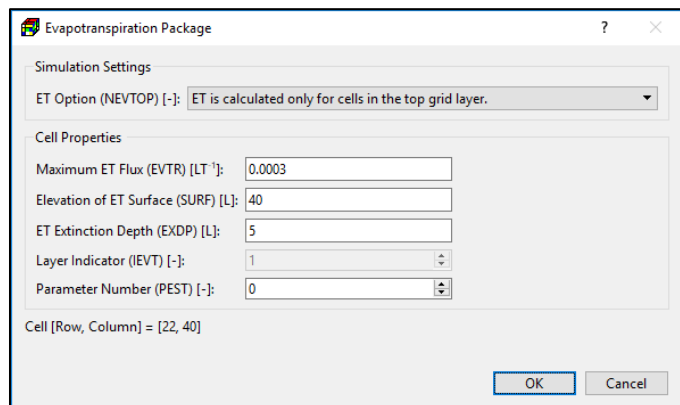
Figure 45. The Evapotranspiration Package dialog box

o   ET is calculated for the highest variable-head cell in each vertical column.

- **Maximum ET Flux (EVTR) [LT^{-1}]:** potential evapotranspiration rate.

- **Elevation of ET Surface (SURF) [L]:** when head is higher than SURF, R_{et} equals to EVTR.

- **ET Extinction Depth (EXDP) [L]:** when head is lower than SURF - EXDP, R_{et} is zero.

- **Layer Indicator (IEVT) [-]:** This indicates the layer from which Q_{et} is removed from the groundwater system.

- **Parameter Number** is used to group cells, where the EVTR value is to be estimated by PEST. See *To define an estimable parameter* in Section 3.8.4 for details.

3.8.1.1.4. Evapotranspiration Segments (ETS1)

The Evapotranspiration Segments (ETS1) Package (Banta, 2000) allows simulation of evapotranspiration with a user-defined relation between evapotranspiration rate and hydraulic head. In the ETS1 Package, the relation of evapotranspiration rate to hydraulic head is conceptualized as a segmented line between an evaporation surface, defined as the elevation where the evapotranspiration rate reaches a maximum, and an elevation located at an extinction depth below the evaporation surface, where the evapotranspiration rate reaches zero. The user supplies input to define as many intermediate segment endpoints as desired to define the relation of evapotranspiration rate to head between these two elevations. The EVT Package, in contrast, simulates evapotranspiration with a single linear function.

The numerical formulation and most required parameters for the ETS Package are the same as those for the EVT Package, other than the segmented function. The required input parameters for all input methods identical and are listed below. Although these parameters are to be assigned to each vertical column of model cells, you may move between layers within the Data Editor to examine the grid configuration in each layer.

1. **All input methods:** Figure 46 shows the dialog box for specifying cell, vertex, or polygon properties.

   - **ET Option (NETSOP) [-]:** Since Q_{et} is calculated for only one cell in each vertical column of model cells, three options are available for specifying the cell where Q_{et} is drawn from:

     o   ET is calculated only for cells in the top grid layer.
     o   ET is calculated for cells in the layers defined by IETS (see below)
     o   ET is calculated for the highest variable-head cell in each vertical column.

   - **Number of Segments [-]:** This is the number of segments of a segmented function that defines the relation of ET rate to hydraulic head. The segmented function is defined by the PXDP and PETM values in the **ET Segment Properties** table below.

- **Maximum ET Flux (ETSR) [LT^{-1}], Elevation of ET Surface (ETSS) [L],** and **ET Extinction Depth (ETSX) [L]:**

  o When the calculated head is higher than ETSS, the ET rate equals to ETSR.

  o When the calculated head is lower than ETSS - EXSS, the ET rate is zero.

  o When the calculated head is below ETSS but the depth of the head below ETSS is less than ETSX, the ET rate is variable and depends on the segmented function defined by the **ET Segment Properties** table below.
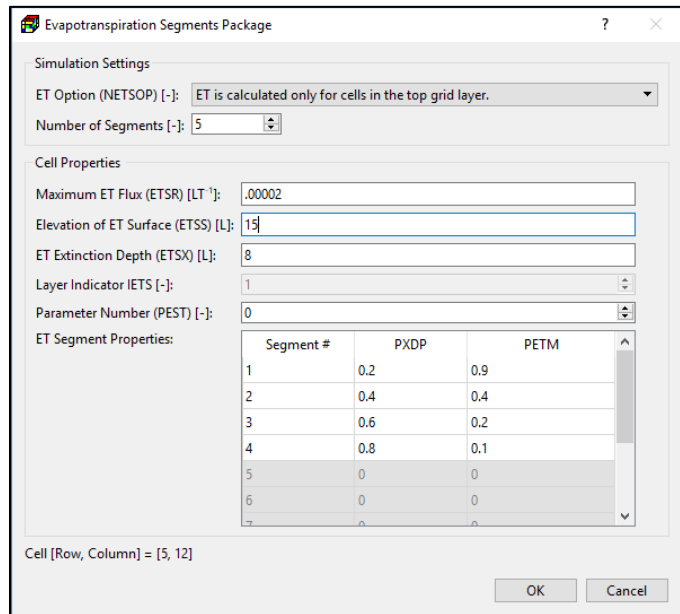
Figure 46. The Evapotranspiration Segments Package dialog box

- **Layer Indicator (IETS) [-]:** This indicates the layer from which Q_{et} is removed from the groundwater system.

- **Parameter Number** is used to group cells, where the ETSR value is to be estimated by PEST. See *To define an estimable parameter* in Section 3.8.4 for details.

- **ET Segment Properties**:

  o **PXDP** is a proportion of the extinction depth (dimensionless), measured downward from the ET surface, which, with PETM, defines the shape of the relation between the evapotranspiration rate and head. PXDP is 0.0 at the ET surface and is 1.0 at the extinction depth. Repetitions of PXDP and PETM are to be specified in sequence such that the first occurrence represents the bottom of the first segment, and subsequent repetitions represent the bottom of successively lower segments. Accordingly, PXDP values for later repetitions (representing lower segments) should be greater than PXDP values for earlier repetitions.

  o **PETM** is a proportion of the maximum evapotranspiration rate (dimensionless) which, with PXDP, defines the shape of the relation between the evapotranspiration rate and head. PETM is 1.0 at the ET surface and is 0.0 at the extinction depth. Repetitions of PXDP and PETM are to be specified in sequence such that the first occurrence represents the bottom of the first segment, and subsequent repetitions represent the bottoms of successively lower segments. Accordingly, PETM values for later repetitions (representing lower segments) generally would be less than PETM values for earlier repetitions.

3.8.1.1.5. Flow and Head Boundary (FHB1)

The Flow and Head Boundary (FHB1) Package (Leake, et al., 1997) allows you to specify flow or head boundary conditions that vary at times other than starting and ending times of stress periods and associated time steps. Values of flow and (or) head at each time step are calculated by linear interpolation of user-specified time-series values. The ability to assign variable flow and head conditions defined at times not corresponding with the model stress periods allows greater flexibility in simulating natural geohydrologic systems and, at the same time, improves the efficiency of the methods used to represent these systems.

The FHB1 Package requires the input of an array of simulation times and for each of the simulation time, the predefined head or flow values at an instance of the FHB1 feature. Multiple instances of FHB1 features may be assigned to a model cell.

The FHB1 Package can be used as an alternative and/or supplement to the Well (WEL) Package or the Recharge (RCH) Package for simulating specified-flow boundaries. FHB1 also is an alternative and/or supplement to the Time-Variant Specified-Head (CHD) Package for simulating specified-head boundaries.

The required input parameters are listed below.

1. **All input methods:** The data entry dialog boxes (Figure 48, Figure 50, Figure 51) of all input methods include a Simulation Settings group that contains the following options:

   - **Times of Specified Values (BDTIM)**: Click the Edit button to open the BDTIM dialog box (Figure 47) where you can edit an array of simulation times at which the flow or head values can be defined. The array of simulation times applies to the entire package. The features of the BDTIM dialog box are as follows:
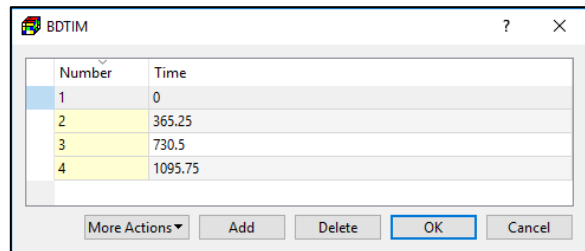
Figure 47. The BDTIM dialog box

     o **Table** contains an array of simulation times.
     o **Add**: Click to add a row to the table.
     o **Delete:** Click to delete the selected row(s) from the table.
     o **More Actions > Save:** Select this item to save the defined simulation times in a Series file (see Section 5.1.13 for its format).
     o **More Actions > Load:** Select this item to clear the table and load simulation times from a Series file.

   - **Include Concentration Data in the SSM Package of MT3D/SEAWAT:** If this box is checked, the values entered to **Concentration (MT3D/SEAWAT) [ML^{-3}]** are associated with the source water. If this box is not checked, the concentration of the source water is assumed to be zero.

1. **Cell-by-cell input method:** Figure 48 shows the dialog box for specifying one or more FHB1 instances to a model cell.

   Figure 48. The Flow and Head Boundary Package dialog box for specifying cell properties

   - **Boundary Type** defines whether the cell represents a specified flow or a specified head boundary, or none.

   - **Cell Face (IAUX)** can be used by programs such as MODPATH (Pollock, 2016) to store information such as the cell face associated with the specified-flow or specified-head boundary.

   - **Time Series of Specified-Flow** or **Time Series of Specified-Head:** The Edit button is activated only if the Boundary Type is Specified-Head or Specified-Flow. Click the Edit button to open the Time Series dialog box (Figure 49) where you can edit an array of specified-flow or specified-head values for the current FHB1 cell instance. The features of the Time Series dialog box are as follows:
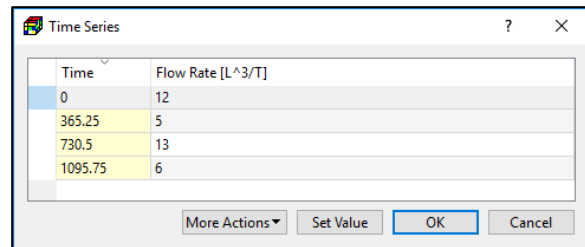
   Figure 49. The Time Series dialog box

   o **Table** contains an array of (read-only) times defined in the BDTIM dialog box and the corresponding flow or head values for the current FHB1 cell instance.
   o **Set Value:** Click to set a uniform head or flow value to the selected row(s) of the table.
   o **More Actions > Save:** Select this item to save the defined flow or head values in a Series file (see Section 5.1.13 for its format).
   o **More Actions > Load:** Select this item to load the flow or head values from a Series file.

   - **Concentration (MT3D/SEAWAT) [ML^{-3}]:** Click the Edit button to open a Concentration dialog box (Figure 42) that allows you to specify the source water concentration of up to 100 species to the current FHB1 instance. The entered concentration values may be used by the SSM Package of MT3D or SEAWAT.

2. **Polyline input method:** Figure 50 shows the dialog box that is used to specify vertex/polyline properties.

   - **Polyline Properties**

o **Boundary Type** defines whether the FHB1 instances in the cells along the polyline represent specified flow or specified head boundary conditions, or none.

o **Cell Face (IAUX)** will be assigned to FHB1 instances in the cells along the polyline. IAUX can be used by programs such as MODPATH (Pollock, 2016) to store information such as the cell face associated with the specified-flow or specified-head boundary.
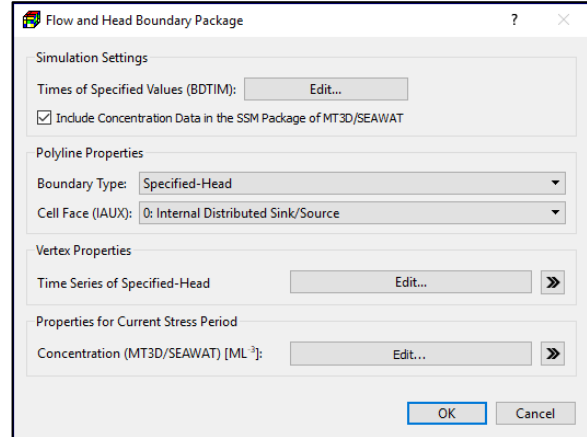
Figure 50. The Flow and Head Boundary Package dialog box for specifying vertex

- **Vertex Properties:** The specified vertex data may be applied to model cells following the rules described in Section 3.3.2.2.

  o **Time Series of Specified-Flow** or **Time Series of Specified-Head:** Click the Edit button to edit an array of specified flow or head values at the current vertex for each of the times defined by BDTIM.

  o **Concentration (MT3D/SEAWAT) [ML^{-3}]:** Click the Edit button to open a Concentration dialog box (Figure 42) that allows you to specify the source water concentration of up to 100 species to the current vertex. The entered concentration values may be used by the SSM Package of MT3D or SEAWAT.

3. **Polygon input method:** Figure 51 shows the dialog box that is used to specify polygon properties. These data may be applied to model cells following the rules described in Section 3.3.2.3.

   - **Polygon Properties**

     o **Boundary Type** defines whether the cells within the polygon represent specified flow or specified head boundary conditions, or none.

     o **Cell Face (IAUX)** will be assigned to cells within the polygon. IAUX can be used by programs such as
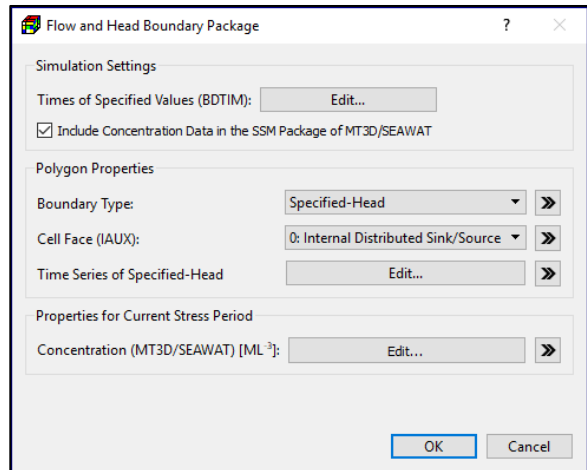
Figure 51. The Flow and Head Boundary Package for specifying polygon properties

MODPATH (Pollock, 2016) to store information such as the cell face associated with the specified-flow or specified-head boundary.

- o **Time Series:** Click the Edit button to edit an array of specified flow or head values at the current vertex for each of the times defined by BDTIM. The specified polygon data are assigned to model cells within the polygon following the rules described in Section 3.3.2.3.
- o **Concentration (MT3D/SEAWAT) [ML^{-3}]:** Click the Edit button to open a Concentration dialog box (Figure 42) that allows you to specify the source water concentration of up to 100 species to the current polygon. The entered concentration values may be used by the SSM Package of MT3D or SEAWAT.

3.8.1.1.6. General-Head Boundary (GHB)

The General-Head Boundary (GHB) Package is used to simulate head-dependent flow boundaries (Cauchy boundary conditions), where flow between an external boundary and the aquifer is at a rate proportional to the head difference between the external boundary and the aquifer.

An external boundary is implemented by dividing into segments so that each segment is completely contained in a single model cell. Multiple external boundary segments may be assigned to a model cell. For each segment, the flow from the external boundary to the cell is calculated by

$$QB = CB \cdot (HB - h) \tag{13}$$

where

QB [L^{3}T^{-1}] is the flow into the cell from the segment of external boundary,

CB [L^{2}T^{-1}] is the boundary conductance of the segment of external boundary,

HB [L] is the head at the segment of external boundary, and

h [L] is the calculated hydraulic head in the cell.

The required input parameters are listed below.

1. **All input methods:** The data entry dialog boxes (Figure 52, Figure 53, and Figure 54) of all input methods include a Simulation Settings group that contains the following option.
   - **Include Concentration Data in the SSM Package of MT3D/SEAWAT:** If this box is checked, the values entered to **Concentration (MT3D/SEAWAT) [ML^{-3}]** are used as source water concentration. If this box is not checked, the concentration of the source water is assumed to be zero.

2. **Cell-by-cell input method:** Figure 52 shows the dialog box for specifying one or more external boundary segments to a model cell. For each segment, the following properties need to be assigned.
   - **Boundary conductance (CB) [L^{2}T^{-1}].** The value of CB depends on the characteristics of the aquifer and the external boundary.

- **Hydraulic Head on Boundary (HB) [L].** This is the head at the segment of external boundary.

- **Parameter Number** is used to group cells, where the CB value is to be estimated by PEST. See *To define an estimable parameter* in Section 3.8.4 for details.

- **GHB Elevation (SEAWAT) [L]:** This is the elevation of the boundary from which the equivalent reference head is calculated. This value is used by

Figure 52. The General-Head Boundary Package dialog box for specifying cell properties

SEAWAT to accurately calculate the flow of variable-density groundwater to the external boundary. The specified value is used only if GHBELEV (in Figure 99) is set as *User-Specified in the GHB Package*.

- **Water Density at GHB (SEAWAT) [L]:** This value is used by SEAWAT and represents the prescribed density of fluid entering the groundwater system from the general-head boundary. This value is used only if SEAWAT is running in the uncoupled mode (i.e., the density-effect of all species are turned off, see Section 3.8.3.1) and GHBDENS (in Figure 99) is set as *User-Specified in the GHB Package*.

- **Concentration (MT3D/SEAWAT) [ML^{-3}]:** Click the Edit button to open a Concentration dialog box (Figure 42) that allows you to specify the source water concentration of up to 100 species. The entered concentration values may be used by the SSM Package of MT3D or SEAWAT.

3. **Polyline input method:** Figure 53 shows the dialog box for specify data to one or more vertices of a polyline.

   - **Simulation Settings**

     o **Auto Layer Number**

       – If this box is checked, the layer number of a segment of external boundary alone the polyline is determined by comparing its *hydraulic head on external boundary (HB)* with the top/bottom elevations of the cells in the same vertical model column as that segment.
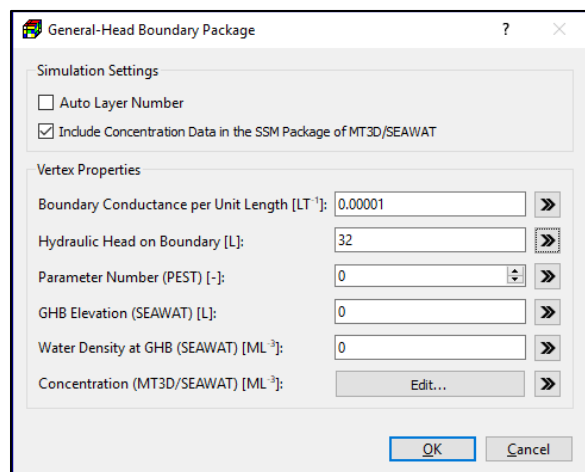
Figure 53. The General-Head Boundary Package dialog for specifying vertex properties.

- if HB is higher than the top elevation of the highest cell, the segment is assigned to the cell in layer 1.
- if HB is lower than the bottom elevation of the lowest cell, the segment is assigned to the cell in layer NLAY.
- If HB lies between top and bottom elevations of a cell, the segment is assigned to that cell.

  – If this box is not checked, the external boundary segments along the polyline are assigned to the layer where the polyline is located.

- **Vertex Properties:** The data of this group are assigned to one or more vertices of a polyline. These vertex data may be interpolated to model cells following the rules described in Section 3.3.2.2 and the rules below.

  o **Boundary conductance per unit length [LT^{-1}]** is interpolated to the cells along the polyline. For each of those cells, the interpolated cell value CB_l is multiplied with the length of the boundary within the cell to obtain the boundary conductance C_d.

  $$CB = CB_l \cdot L_c \qquad\qquad (14)$$

  where

  CB_l is the boundary conductance per unit length at a given cell, and

  L_c is the length of the boundary within the cell.

- **All other parameters**: Refer to the cell-by-cell input method above for the descriptions of these parameters.

4. **Polygon input method:** Figure 54 shows a dialog box for specify the following data to a polygon. These data may be applied to model cells following the rules described in Section 3.3.2.3 and additional rules below.

- **Simulation Settings:** See the description for the polyline input method above.

- **Polygon Properties:**

  o **Boundary conductance per unit area [T^{-1}].** For each cell within the polygon, the specified value (CB_a) is multiplied with the cell area to obtain the boundary conductance CB.
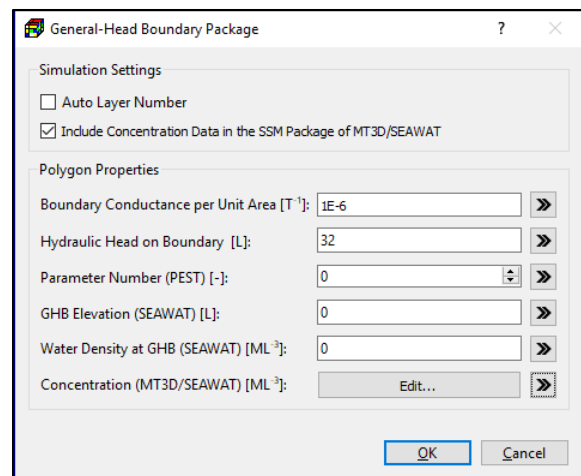
Figure 54. The General-Head Boundary Package dialog for specifying polygon properties.

$$CB = CB_a \cdot Area_c \qquad\qquad (15)$$

where

CB_a is the boundary conductance per unit area [T^{-1}], and

$Area_c$ is the area of the cell.

○ **The other parameter:** Refer to the cell-by-cell input method above for the descriptions of these parameters.

3.8.1.1.7. Horizontal-Flow Barrier (HFB6)

The Horizontal-Flow Barrier (HFB6) Package simulates thin low-permeability geologic features, such as vertical faults or slurry walls, which impede the horizontal flow of groundwater. These geologic features are approximated as a series of horizontal-flow barriers conceptually situated on the boundaries between pairs of adjacent cells in the finite-difference grid. The Horizontal-Flow Barrier was developed by (Hsieh, et al., 1993) and has been incorporated into MODFLOW–2005 and renamed to HFB6.

Horizontal-flow barriers are defined by assigning the following values to model cells with the cell-by-cell input method. The polyline and polygon input methods are not supported.

1. **Cell-by-cell input method:** Figure 55 shows the dialog box for specifying cell properties.

   • **Hydraulic characteristic** is the hydraulic conductivity of the barrier divided by the thickness of the barrier.
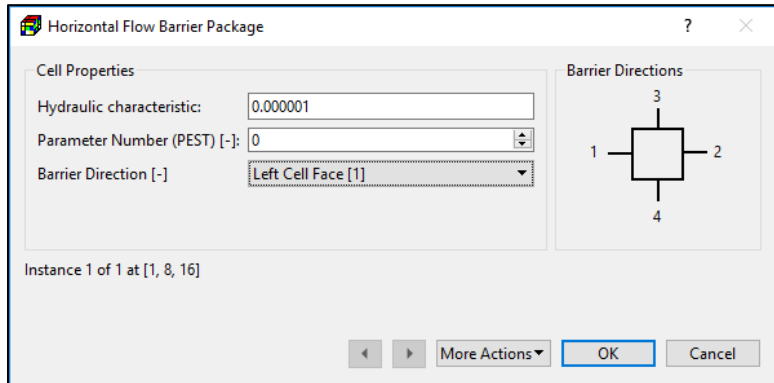
Figure 55. The Horizontal Flow Barrier Package dialog box

   • **Parameter Number** is used to group cells, where the hydraulic characteristic value is to be estimated by PEST. See *To define an estimable parameter* in Section 3.8.4 for details.

   • **Barrier Direction [-]:** The barrier direction indicates the cell face where the barrier is located. To erase an existing barrier, select *No Barrier [0]*.

2. **Polyline and Polygon input methods** are not supported.

3.8.1.1.8. Interbed Storage (IBS)

The Interbed Storage (IBS) Package (Leake, et al., 1991) may only be used in a transient flow simulation. For steady state flow simulations, this menu item is deactivated.

Removal of ground water by pumping from aquifers may result in compaction of compressible fine-grained beds that are within or adjacent to the aquifers. Compaction of the sediments and resulting land subsidence may be permanent if the head declines result in vertical stresses

beyond the previous maximum stress. IBS is designed to simulate storage changes from both elastic and inelastic compaction. In IBS, elastic compaction or expansion is assumed to be proportional to change in head. The constant of proportionality is the product of the skeletal component of elastic specific storage and the thickness of the sediments. Similarly, inelastic compaction is assumed to be proportional to decline in head. The constant of proportionality is the product of the skeletal component of inelastic specific storage and the thickness of the sediments. Within a model time step, IBS appropriately apportions storage changes between elastic and inelastic components based on the relation of simulated head to the previous minimum (preconsolidation or critical) head.

The required input parameters for all input methods are identical and listed below.

1. **All input methods:** Figure 56 shows the dialog box for specifying cell, vertex, or polygon properties.

   • **Data Tab**

     o **Preconsolidation Head (HC) or Critical Head [L]:** Preconsolidation head is the previous minimum head value in the aquifer. For any model cells in which the specified preconsolidation head is greater than the initial

Figure 56. The Interbed Storage Package dialog box

hydraulic head, the value of the preconsolidation head will be set to that of the initial hydraulic head; When compressible fine-grained sediments are stressed beyond a previous maximum stress (preconsolidation stress), compaction is permanent (inelastic).

     o **Elastic Storage Factor (Sfe) [-]:** IBS uses the following equation to calculate the change in the thickness Δb [L] of the interbed (positive for compaction and negative for expansion):

$$\Delta b = -\Delta h \cdot Sfe \tag{16}$$

where

Δh [L] change in hydraulic head, positive for increase.

     o **Inelastic Storage Factor (Sfv) [-]:** IBS uses the following equation to calculate the change in the thickness Δb [L] of the interbed (positive for compaction and negative for expansion):

$$\Delta b = -\Delta h \cdot Sfv \tag{17}$$

- o **Starting Compaction (COM) [L]:** Compaction values computed by the IBS package are added to the starting compaction so that stored values of compaction and land subsidence may include previous components. The starting compaction does not affect the calculation of storage changes or resulting compaction.
- o **Parameter Number** is used to group cells, where the value of the inelastic storage factor is to be estimated by PEST. See *To define an estimable parameter* in Section 3.8.4 for details.

- **Options Tab**: The following optional output are available. Check the corresponding box to include the output values in the modflow.interbed file.

  - o Subsidence
  - o Compaction of Individual Layers
  - o Preconsolidation Heads

3.8.1.1.9. Lake (LAK3)

The Lake (LAK3)[33] Package (Merritt, et al., 2000) simulates stationary surface-water bodies (lakes) that are in direct contact with the aquifer. A lake is represented as a volume of space within the model grid which consists of inactive cells extending downward from the upper surface of the grid. Active model grid cells bordering this space, representing the adjacent aquifer, exchange water with the lake at a rate determined by the relative heads and by conductances that are based on grid cell dimensions, hydraulic conductivities of the aquifer material, and user-specified leakance distributions that represent the resistance to flow through the material of the lakebed. Parts of the lake may become "dry" as upper layers of the model are dewatered, with a concomitant reduction in lake surface area, and may subsequently rewet when aquifer heads rise. An empirical approximation has been encoded to simulate the rewetting of a lake that becomes completely dry.

The variations of lake stages are determined by independent water budgets computed for each lake in the model grid. This lake budget process makes the package a simulator of the response of lake stage to hydraulic stresses applied to the aquifer. Implementation of a lake water budget requires input of parameters including those representing the rate of lake atmospheric recharge and evaporation, overland runoff, and the rate of any direct withdrawal from, or augmentation of, the lake volume. The lake/aquifer interaction may be simulated in both transient and steady-state flow conditions, and the user may specify that lake stages be computed explicitly, semi-implicitly, or fully implicitly in transient simulations.

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[33] MODFLOW-2005 will not work if the LAK3 Package is activated and the LAK box of Modflow Output Control (Section 3.8.1.3) is checked. If the LKT Package of MT3D-USGS is not used, uncheck the LAK box. If you need to use the LKT Package, the LAK box must be checked and you must use MODFLOW-NWT for the flow simulation by either setting the UPW package as the internal flow package (Section 3.4.6) or assigning the executable of MODFLOW-NWT to the path of MODFLOW-2005 in Preferences (Section 3.4.11).

Because lakes with irregular bathymetry can exist as separate pools of water at lower stages, that coalesce to become a single body of water at higher stages, logic was added to the Lake Package to allow the representation of this process as a user option. If this option is selected, a system of linked pools (multiple-lake system) is identified in each time step and stages are equalized based on current relative sublake surface areas.
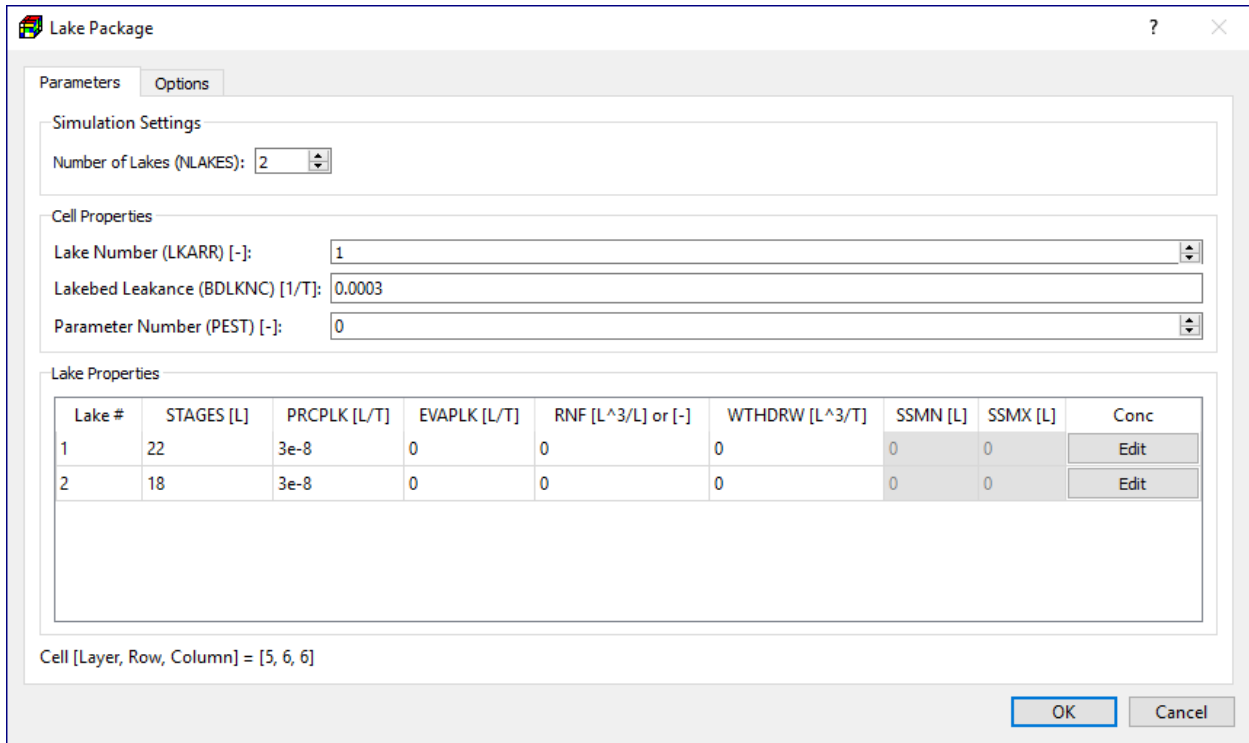
Figure 57. The Lake Package dialog box

Lake cells are defined with the cell-by-cell input method. The polyline and polygon input methods are not supported.

1. **Cell-by-cell input method:** Figure 57 shows the dialog box for specifying cell properties.

   - **Parameters Tab**

     o **Simulation Settings**

       – **Number of Lakes (NLAKES) [-]:** This is the number of lakes to be simulated throughout the entire simulation. Sublakes of multiple-lake systems (see *Options Tab* below) are considered separate lakes for input purposes.

     o **Cell Properties:** This group define the properties of the lake cell for the current stress period.

       – **Lake Number (LKARR) [-]:** This is the identification number of the lake occupying the grid cell. The lake number must be positive and must not exceed NLAKES. A lake must be in a grid cell that meets the following requirements:

- The cell must be a no-flow cell (i.e., IBOUND = 0)
- The cell must not be re-wettable (see Section 3.8.1.1.21).
- The cell may not be overlain by non-lake cells.

  - **Lakebed Leakance (BDLKNC) [1/T]:** This is the lakebed leakance that will be assigned to lake/aquifer interfaces that occur in the corresponding grid cell.
  - **Parameter Number (PEST) [-]** is used to group cells, where the BDLKNC value is to be estimated by PEST. See *To define an estimable parameter* in Section 3.8.4 for details.

o **Lake Properties:** This table define the hydrologic properties of individual lakes for the current stress period.

  - **Lake #:** This is the identification number of a lake.
  - **Stages [L]:** Initial stage of the lake at the beginning of the simulation.
  - **PRCPLK [L/T]:** The rate of precipitation per unit area at the surface of the lake.
  - **EVAPLK [L/T]:** The rate of evaporation per unit area from the surface of the lake.
  - **RNF [L³/L] or [-]:** Overland runoff from an adjacent watershed entering the lake.

    - If RNF > 0, it is specified directly as a volumetric rate [L³/T].
    - If RNF < 0, its absolute value is used as a multiplier applied to the product of PRCPLK and the surface area of the lake at its full stage.

  - **WTHDRW [L^3/T]:** The volumetric rate of water removal from the lake by means other than rainfall, evaporation, surface outflow, or groundwater seepage. A negative value indicates augmentation.
  - **SSMN [L]:** Minimum stage allowed for the lake in steady-state simulation.
  - **SSMX [L]:** Maximum stage allowed for the lake in steady-state simulation.
  - **Conc:** Click the *Edit* button to open the Lake Concentration dialog box that allows you to specify the initial concentration values, and concentration values associated with the precipitation and runoff of up to 100 species for the lake.

    - The concentration values specified in the Lake Concentration dialog box are used only by the LKT Package of MT3D-USGS.
    - If the LKT Package is not activated or if you are using MT3DMS or SEAWAT, you may use Models > MT3DMS/SEAWAT > Package > Sink/Source Mixing (SSM) > Lake (LAK) to specify the concentration values of the lake water.

- **Options Tab (**Figure 58**)**

o **Solution Parameters:** These parameters are defined for the entire simulation.

  - **Time-Weighting Factor (THETA) [-]:** THETA is automatically set to a value of 1.0 for all steady-state stress periods. For transient stress periods,
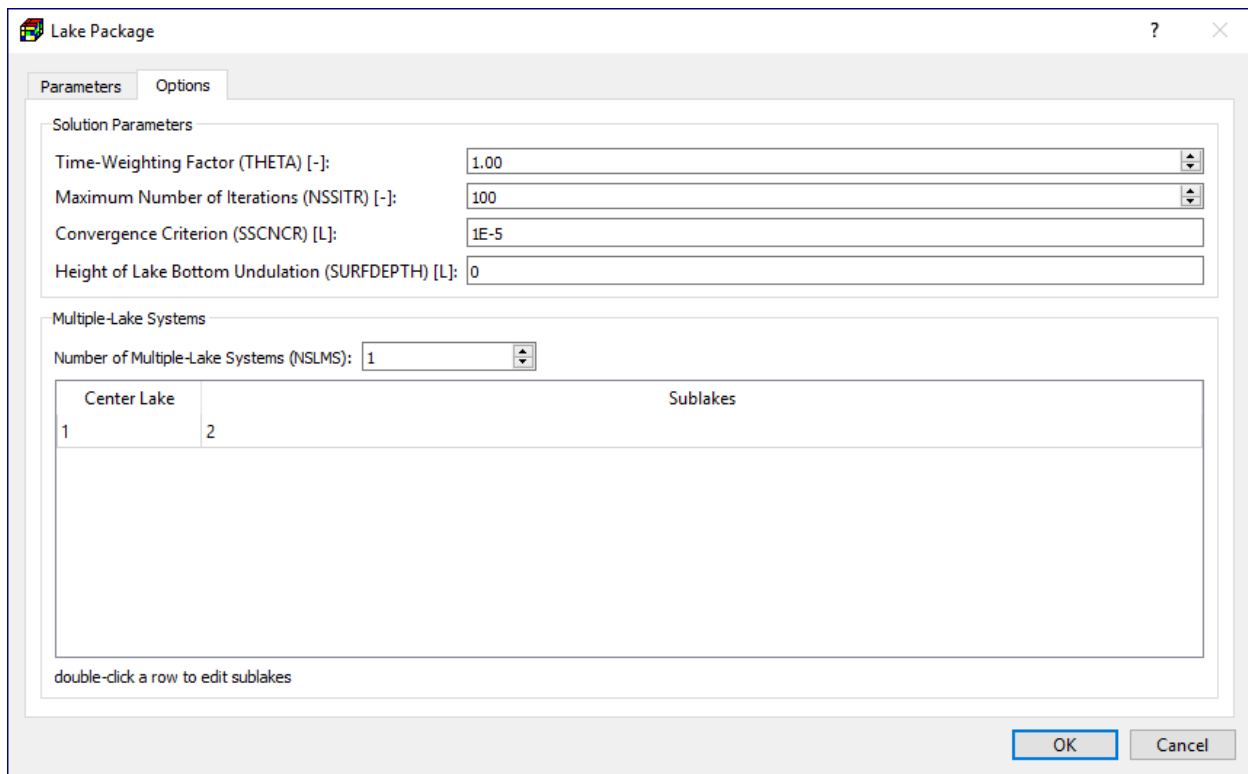
Figure 58. The Options tab of the Lake Package dialog box

- **0.0 ≤ THETA ≤ 0.5**: Explicit solution for lake stages.
- **0.5 < THETA < 1.0**: semi-implicit solution for lake stages
- **THETA = 1.0:** implicit solution for lake stages.

- **Maximum Number of Iterations (NSSITR) [-]:** Maximum number of iterations for the solution for equilibrium lake stages in each MODFLOW iteration for steady-state aquifer head solution.
- **Convergence Criterion (SSCNCR) [L]:** Convergence criterion for equilibrium lake stage solution by Newton's method.
- **Height of Lake Bottom Undulation (SURFDEPTH) [L]:** SURFDEPTH provides a smooth transition for lakes between dry and wet, and thus reduces numerical oscillations. Values of SURFDEPTH ranging from 0.01 to 0.5 have been used successfully in test simulations.

o **Multiple-Lake Systems:** This group define the properties of the multiple-lake systems for the current stress period.

- **Number of Multiple-Lake Systems (NSLMS):** The number of multiple-lake systems if coalescing/dividing lakes are to be simulated (only in transient runs). Enter 0 if no multiple-lake systems are to be simulated.
- **Table**: Each row of the table represents a multiple-lake system. The Center Lake column lists the lake identification number of the center lake of the system; the

Sublakes column lists the lake identification numbers of sublakes of the system. Double-click a row to edit the multiple-lake system in the Multiple-Lake System dialog box (Figure 59). The items of the dialog box are as follows:

- **Center Lake #:** This is the lake identification number of center lake of the multiple-lake system.
- **Number of Sublakes:** This is the number of sublakes of the multiple-lake system.
- **Lake #:** This is the lake identification number of a given sublake.
- **Sillvt [L]:** This is the sill elevation, defined as the elevation at which the center lake and the given sublake are connected and have a common state and water budget.
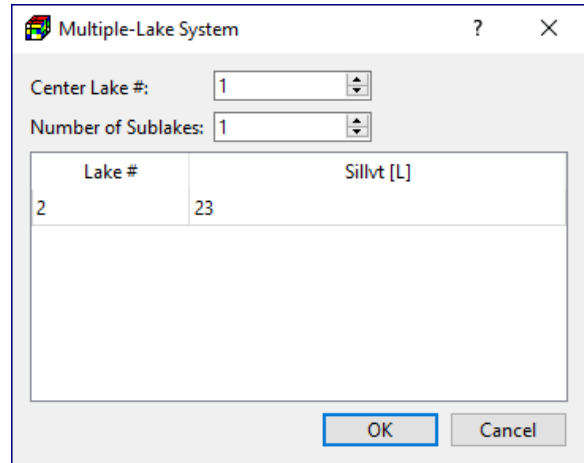
Figure 59. The Multiple-Lake System dialog box

3.8.1.1.10. Multi-Node Well (MNW1)

The Multi-Node Well[32] (MNW1) Package (Halford, et al., 2002) allows you to simulate wells that extend beyond a single model node (i.e., model cell). Multi-node wells can simulate wells that are completed in multiple aquifers or in a single heterogeneous aquifer, partially penetrating wells, and horizontal wells. Multi-aquifer wells dynamically distribute flow between nodes under pumping, recharging, or unpumped conditions. Variations in intra-borehole flow can be simulated with the MNW1 Package, which is limited by how finely an aquifer system has been discretized vertically. Simulated discharge from single-node and multi-node wells also can be drawdown limited, which is user specified for pumping or recharging conditions. The MNW1 Package can track potential mixes of a water-quality attribute.

A MNW1 well is defined by assigning the following values to a model cell with the cell-by-cell input method. The polyline and polygon input methods are not supported.

1. **Cell-by-cell input method:** Figure 60 shows the dialog box for specifying cell properties.
   - **Parameters Tab**
     o **Well Loss Type [-]:** This is the model for well loss. The selected Loss Type applies to all MNW1 wells.
     o **Exponent P [-]** is the power (exponent) of the nonlinear discharge component of well loss and is used only when Loss Type is Nonlinear. The specified value of P applies to all MNW1 wells.
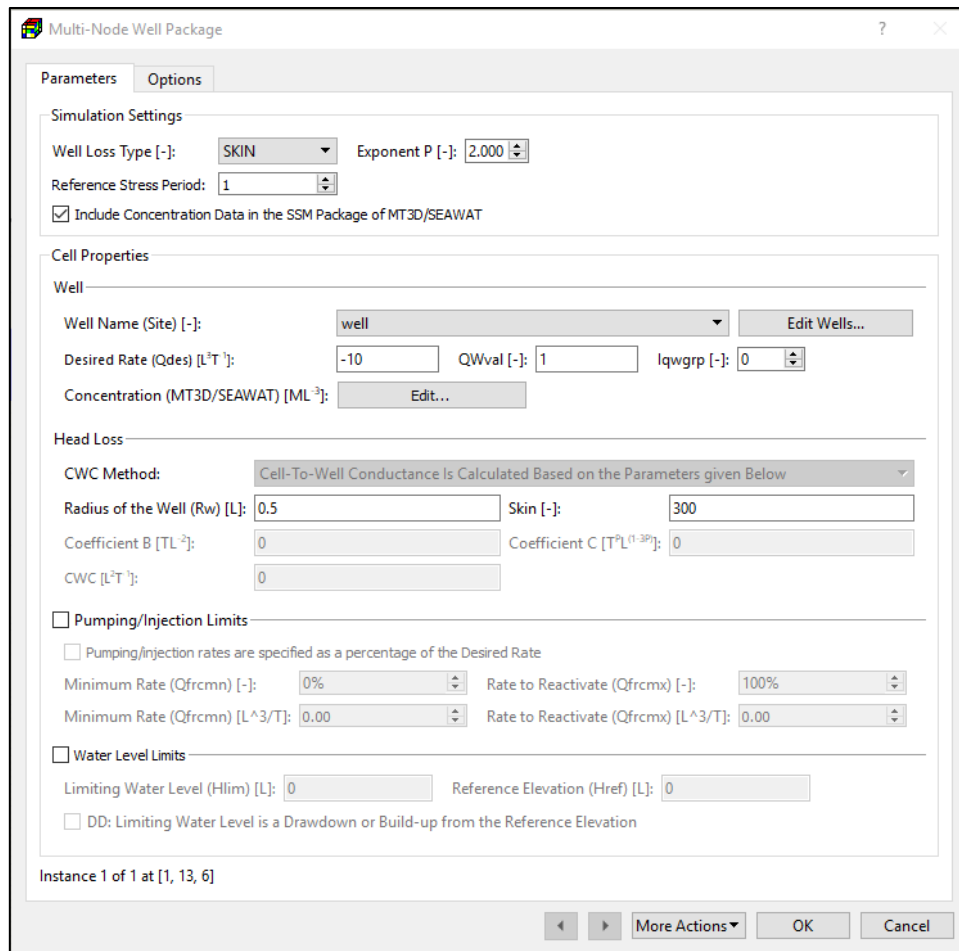
Figure 60. The Multi-Node Well Package dialog box

o **Reference Stress Period (*kspref*):** The hydraulic head at the beginning of the reference stress period will be used as the reference values for calculating drawdown. See *Limiting Water Level (Hlim)* below for details.

o **Include Concentration Data in the SSM Package of MT3D/SEAWAT:** If this box is checked, the values entered to **Concentration (MT3D/SEAWAT) [ML^{-3}]** are associated with the source water. If this box is not checked, the concentration of the source water is assumed to be zero.

o **Well**

– **Edit Wells:** Click this button to open the MNW1 Wells dialog box that allows you to edit wells.

– **Well Name (Site) [-]:** Select an existing well to which the following values apply.

– **Desired Rate (Qdes) [L^{3}T^{-1}]:** The desired injection or extraction rate of the well. Enter a positive value for injection; a negative value for extraction.

– **QWval [-]:** Water-quality value that is to be flow-rate averaged amongst wells in the same Iqwgrp.

- **Iqwgrp [-]:** Water quality group identifier. Flow-rate averaged water-quality values are reported for wells within the same Iqwgrp.
- **Concentration (MT3D/SEAWAT) [ML^{-3}]:** Click the Edit button to open a Concentration dialog box (Figure 42) that allows you to specify the injected water concentration of up to 100 species. The entered concentration values are used by the SSM Package of MT3D or SEAWAT.

o **Head Loss**

- **CWC Method:** Specify how the value of Cell-to-Well Conductance (CWC) is determined. For multi-node wells, CWC Method must be "Cell-to-well conductance is calculated based on the parameters given below".
- **Radius of the Well (Rw) [L]:** Rw is used to calculate the cell-to-well conductance as formulated by (Peaceman, 1983).
- **Skin [-]** defines the friction losses to the well owing to the screen and to formation damage. This value is used only if the Loss Type is Skin.
- **Coefficient B [TL^{-2}]:** This is the coefficient B of the general well-loss equation and is used only when the Loss Type is Linear or Nonlinear. The coefficient B accounts for head losses that occur adjacent to and within the borehole and well.
- **Coefficient C [$T^{P}L^{(1-3P)}$]:** This is the coefficient C accounting for the nonlinear well-loss due to turbulent flow near the well. P is the power (exponent) of the nonlinear discharge component of well loss. The coefficient C is used only when the Loss Type is Nonlinear.
- **CWC [$L^{2}T^{-1}$]:** This value is the specified cell-to-well conductance.

o **Pumping/Injection Limits**

- **Limits are specified as a percentage of the Desired Rate:** If this box is checked, pumping/injection limits are specified as a percentage of the *Desired Rate (Qdes)*. If this box is not checked, pumping/injection limits are specified as a rate in the unit of [L^3/T].
- **Minimum Rate (Qfrcmn) [-]:** The minimum rate (as a percentage of *Qdes*) that a well must exceed to remain active.
- **Rate to Reactivate (Qfrcmx) [-]:** The minimum potential rate (as a percentage of *Qdes*) that must be exceeded to reactivate a well.
- **Minimum Rate (Qfrcmn) [L^3/T]:** The minimum rate that a well must exceed to remain active.
- **Rate to Reactivate (Qfrcmx) [L^3/T]:** The minimum potential rate that must be exceeded to reactivate a well.

- o **Water Level Limits**

    - **Limiting Water Level (Hlim) [L]:** this value constrains the pumping/injection rate.

        - If the *DD* box (see below) is not checked,
            a. *Hlim* is the minimum water level for *Qdes* < 0, and
            b. *Hlim* is the maximum water level for *Qdes* > 0.

        - If the *DD* box is checked,
            a. [*Href – Hlim*] is the minimum water level for *Qdes* < 0, and
            b. [*Href + Hlim*] is the maximum water level for *Qdes* > 0.

    - **Reference Elevation (Href) [L]:** If the specified value of Href is greater than the maximum hydraulic head value of the *Reference Stress Period (kspref)*, Href is set to the simulated hydraulic head value at the location of the well.
    - **DD: Limiting Water Level Is a Drawdown or Build-up from the Reference Elevation:** the status of this box affects how the limiting water level is defined. See *Limiting Water Level (Hlim)* above for details.

- **Options Tab**

    - o **BYNODE:** if this box is checked, a file with the specified **File Name** will be created. This file stores flow rates of each node of the multi-node wells.
    - o **QSUM:** if this box is checked, a file with the specified **File Name** will be created. This file stores the water level and the sum of flow rates of each multi-node well.
    - o If both boxes of **BYNODE** and **QSUM** are checked, additional output files will be created for each individual multi-node wells. The filename for a well will be composed of the prefix "MNW1Output.", the well name, and the suffix ".txt". For example, if the well name is "Well-A", the output file will be named as "MNW1Outout.Well-A.txt". Each of those output files will contain time-series of discharge, water level in well, average water-quality value (based on QWval) of the specific well, as well as the flow rates of all nodes of that well.

2. **Polyline and Polygon input methods** are not supported.

3.8.1.1.11. Recharge (RCH)

The Recharge (RCH) Package is designed to simulate distributed recharge to the ground-water system. The RCH Package does not allow for recharge to occur simultaneously at multiple depths in the same vertical column because natural recharge enters the ground-water system at the top, and therefore a value of the recharge flux RECH [LT^{-1}] is assigned to a cell in each vertical column of model cells. The recharge rate to the groundwater system Q_{rch} [L^{3}T^{-1}] is calculated by

$$Q_{rch} = RECH \cdot Area_c \qquad\qquad (18)$$

where

$RECH$ [LT^{-1}] is the recharge flux at the cell, and

$Area_c$ is the area of the cell.

The required input parameters for all input methods are identical and listed below. Although these parameters are to be assigned to each vertical column of model cells, you may move between layers within the Data Editor to examine the grid configuration in each layer.

1. **All input methods:** Figure 61 shows the dialog box for specifying cell, vertex, or polygon properties.

   - **Recharge Option (NRCHOP) [-]:** Since Q_{rch} is calculated for only one cell in each vertical column of model cells, three options are available for specifying the cell where Q_{rch} is applied to:
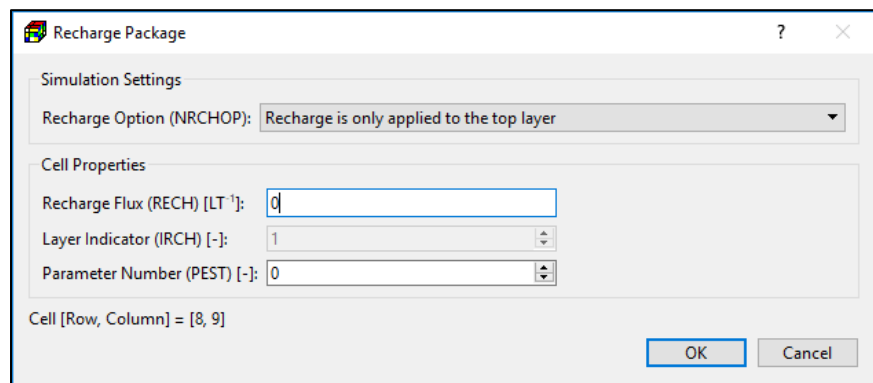
Figure 61. The Recharge Package dialog box

   o Recharge is only applied to the top layer.
   o Vertical distribution of recharge is specified in IRCH
   o Recharge is applied to the highest variable-head cell in each vertical column

   - **Recharge Flux (RECH) [LT^{-1}].**

   - **Layer Indicator (IRCH) [-]:** This indicates the layer from which Q_{rch} is added to the groundwater system.

   - **Parameter Number** is used to group cells, where the RECH value is to be estimated by PEST. See *To define an estimable parameter* in Section 3.8.4 for details.

3.8.1.1.12. River (RIV)

The purpose of the River (RIV) Package is to simulate the effects of flow between surface-water features and groundwater systems. Rivers and streams contribute water to or drain water from the groundwater system, depending on the head gradient between the river and the ground-water regime.

A river is implemented by dividing into reaches so that each reach is completely contained in a single model cell. Multiple reaches may be assigned to a model cell. For each reach, the flow rate Q_{riv} [L^{3}T^{-1}] between the reach and the model cell is calculated by the following equations.

$$Q_{riv} = C_{riv} \cdot (h_{riv} - h) \qquad \text{if } h > B_{riv} \tag{19}$$

$$Q_{riv} = C_{riv} \cdot (h_{riv} - B_{riv}) \quad \text{if } h < B_{riv} \tag{20}$$

where

Q_{riv} [L^{3}T^{-1}] is the flow rate between the reach and the model cell (i.e., the groundwater system). A positive value means that water flows from the river to aquifer,

h [L] is the calculated hydraulic head in the cell containing the reach,

h_{riv} [L] is the head in the reach,

B_{riv} [L] is the elevation of the riverbed bottom of the reach, and

C_{riv} [L^{2}T^{-1}] is the riverbed conductance of the reach.

The required input parameters are listed below.

1. **All input methods**: The data entry dialog boxes of all input methods include a Simulation Settings group that contains the following option.

    - **Include Concentration Data in the SSM Package of MT3D/SEAWAT:** If this box is checked, the values entered to **Concentration (MT3D/SEAWAT) [ML^{-3}]** are used as source water concentration. If this box is not checked, the concentration of the source water is assumed to be zero.

2. **Cell-by-cell input method:** Figure 62 shows the dialog box for specifying one or more reaches to a model cell. For each reach, the following properties need to be assigned.

    - **Riverbed conductance C_{riv} [L^{2}T^{-1}]** relates flow rate to the head differences between the reach and the aquifer. The value of C_{riv} depends on the material and characteristics of the riverbed and the immediate environment.

    - **River Stage h_{riv} [L]** is the hydraulic head of the reach.

    - **Elevation of the Riverbed Bottom (B_{riv}) [L]** is the elevation of the bottom of the riverbed.
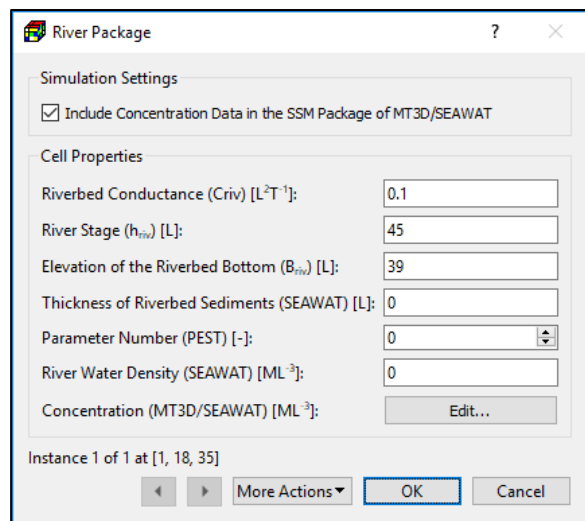
Figure 62. The River Package dialog box for specifying cell properties

- **Parameter Number** is used to group cells, where the C_{riv} value is to be estimated by PEST. See *To define an estimable parameter* in Section 3.8.4 for details.

- **Thickness of Riverbed Sediments (SEAWAT) [L]:** This value is used by SEAWAT to appropriately include the effects of variable-density river leakage and is used only if RBDTHK (in Figure 99) is set as *User-Specified in the RIV Package*.

- **River Water Density (SEAWAT) [ML⁻³]** is the water density of the river. This is used by SEAWAT only if it is running in the uncoupled mode (i.e., the density-effect of all species are turned off, see Section 3.8.3.1) and RIVDEN (in Figure 99) is set as *User-Specified in the RIV Package*.

- **Concentration (MT3D/SEAWAT) [ML⁻³]:** Click the Edit button to open a Concentration dialog box (Figure 42) that allows you to specify the source water concentration of up to 100 species to the river. The entered concentration values may be used by the SSM Package of MT3D or SEAWAT.

3. **Polyline input method:** Figure 63 shows a dialog box for specify data to one or more vertices of a polyline. The specified vertex data may be interpolated to model cells following the rules described in Section 3.3.2.2 and the rules below.

   - **Simulation Settings**

     o **Auto Layer Number**

       – If this box is checked, the layer number of a reach alone the polyline is determined by comparing its elevation of the riverbed bottom (B_{riv}) with the top/bottom elevations of the cells in the same vertical model column as the reach.

Figure 63. The River Package dialog box for specifying vertex properties

   - if B_{riv} is higher than the top elevation of the highest cell, the reach is assigned to the cell in Layer 1.
   - if B_{riv} is lower than the bottom elevation of the lowest cell, the reach is assigned to the cell in Layer NLAY.
   - If B_{riv} lies between top and bottom elevations of a cell, the reach is assigned to that cell.

       – If this box is not checked, the reaches along the polyline are assigned to the layer where the polyline is located.

- **Vertex Properties:** The data of this group are assigned to one or more vertices of a polyline. These vertex data may be interpolated to model cells following the rules described in Section 3.3.2.2 and the rules below.

  - **Riverbed conductance per unit length C_{rivl} [LT⁻¹]** is interpolated to the cells along the polyline. For each of those cells, the interpolated cell value C_{rivl} is multiplied with the length of the river within the cell to obtain the riverbed conductance C_{riv}:

$$C_{riv} = C_{rivl} \cdot L_c \qquad\qquad (21)$$

    where

    C_{rivl} is the riverbed conductance per unit length at a given cell, and

    L_c is the length of the river within the cell.

  - **All other parameters:** Refer to the cell-by-cell input method above for the descriptions of these parameters.

4. **Polygon input method:** Figure 64 shows a dialog box for specify the following data to a polygon. These data may be applied to model cells following the rules described in Section 3.3.2.3 and additional rules below.

   - **Simulation Settings:** See the description for the polyline input method above.

   - **Polygon Properties**

     - **Riverbed conductance per unit area C_{riva} [T⁻¹].** For each cell within the polygon, the specified value (C_{riva}) is multiplied with the cell area to obtain the riverbed conductance C_{riv}:

Figure 64. The River Package dialog box for specifying polygon properties

$$C_{riv} = C_{riva} \cdot Area_c \qquad\qquad (22)$$

       where

       C_{riva} is the riverbed conductance per unit area, and

       $Area_c$ is the area of the cell.

     - **The other parameters:** Refer to the cell-by-cell input method above for the descriptions of these parameters.

3.8.1.1.13. Reservoir (RES1)

The Reservoir (RES1) Package (Fenske, et al., 1996) simulates leakage between a reservoir and an underlying groundwater system as the reservoir area expands and contracts in response to changes in reservoir stage. The Reservoir Package also automates the process of specifying head-dependent boundary cells during the simulation. For each time step, all cells for which the reservoir stage is above the reservoir land-surface elevation are simulated as active reservoir cells. Leakage between the reservoir and the underlying groundwater system is simulated for each active reservoir cell by multiplying the difference between the reservoir stage and the groundwater head by the hydraulic conductance of the reservoir bed. The package uses linear interpolation to calculate reservoir stage for each time step within a stress period.

The flow rate Q_{res} [L³T⁻¹] between the reservoir and the underlying groundwater system is simulated for each vertical column of model cells corresponding to the inundated area of the reservoir with the following equations.

$$Q_{res} = C_{res} \cdot (h_{res} - h) \qquad if \; h > B_{res} - Rbthck \qquad (23)$$

$$Q_{res} = C_{res} \cdot (h_{res} - B_{res}) \quad if \; h < B_{res} - Rbthck \qquad (24)$$

where

> Q_{res} [L³T⁻¹] is the flow rate between the reservoir and the model cell (i.e., the groundwater system) to which the reservoir is connected (see connection option below). A positive value means that water flows from the reservoir to the groundwater system,
>
> C_{res} [L²T⁻¹] is the reservoir-bed conductance,
>
> h_{res} [L] is the reservoir stage,
>
> h [L] is the calculated hydraulic head in the connected model cell,
>
> B_{res} [L] is the land surface elevation (i.e., elevation of the top of reservoir-bed), and
>
> $Rbthck$ [L] is the thickness of the reservoir-bed.

The reservoir-bed conductance C_{res} [L²T⁻¹] is calculated by

$$C_{res} = HC_{res} \cdot Area_c \; / \; Rbthck \qquad (25)$$

where

> HC_{res} [LT⁻¹] is the vertical hydraulic conductivity of the reservoir-bed sediments, and
>
> $Area_c$ is the area of the connected cell.

Inherent in the simulation of reservoirs is that the reservoir only partially penetrates an active model cell. If the reservoir fully penetrates a cell, it is assumed that the cell will be specified as no flow and that reservoir flow will be simulated in a lower cell. Thus, water exchange between

the ground-water system and the reservoir takes place across the bottom of the reservoir. Refer to p. 4 of (Fenske, et al., 1996) for details.

A reservoir is defined by assigning the following values to each vertical column of model cells with the cell-by-cell or polygon input methods. The polyline input method is not supported. Figure 65 shows the dialog box for specifying cell properties. Although these parameters are to be assigned to each vertical column of model cells, you may move between layers within the Data Editor to examine the grid configuration in each layer.

1. **All supported input methods**

   - **Layer Connection Options:** Define how and where the reservoir leakage is connected to the groundwater system. The connection options apply to all reservoirs. The following options are available.

     o Reservoirs are connected to the top layer
     o Reservoirs are connected to the highest variable-head cells (of each vertical column of model cells.)

Figure 65. The Reservoir Package dialog box

     o Reservoirs are connected to the layers defined by IRESL.

   - **Include Concentration Data in the SSM Package of MT3D/SEAWAT:** If this box is checked, the values entered to **Concentration (MT3D/SEAWAT) [ML^{-3}]** are used as source water concentration. If this box is not checked, the concentration of the source water is assumed to be zero.
   - **Layer Number (IRESL) [-]:** Defines the layer to which the current reservoir cell is connected. Required only if the third connection option is selected.

   - **Reservoir Number (IRES) [-]:** The number of the reservoir to which the vertical column of cells is connected. A value of zero or less indicates the absence of reservoirs at the corresponding cell location. Values greater than zero indicate that the cell is part of the corresponding reservoir.

   - **Land Surface Elevation (Bres) [L]:** The land surface elevation within the specified area of potential inundation for each reservoir is typically defined by the average land surface elevation of individual cells within the area. At cells in which reservoir stage exceeds Bres, the reservoir boundary is activated. Similarly, wherever reservoir stage is less than Bres, the reservoir boundary is not activated.

   - **Vertical Hydraulic Conductivity (HCres) [LT^{-1}]:** This is the vertical hydraulic conductivity of the reservoir bed overlying the current cell.

- **Reservoir Bed Thickness (Rbthck) [L]:** This is the thickness of the reservoir-bed sediments overlying the current cell.

- **Parameter Number** is used to group cells, where the HCres value is to be estimated by PEST. See *To define an estimable parameter* in Section 3.8.4 for details.

- **Concentration (MT3D/SEAWAT) [ML^{-3}]:** Click the Edit button to open a Concentration dialog box (Figure 42) that allows you to specify the source water concentration of up to 100 species. The entered concentration values may be used by the SSM Package of MT3D or SEAWAT.

- **Stage:** Click this button to open the Reservoir Stage Time Series dialog box (Figure 66) for specifying the water table elevations of reservoirs.

  - **Reservoir table:** Select a reservoir number (a row) from the Reservoir table. The reservoir number is corresponding to IRES (see above). You can optionally assign the names of the reservoirs to the Name column.

  - **Stage Table:** Enter the observation
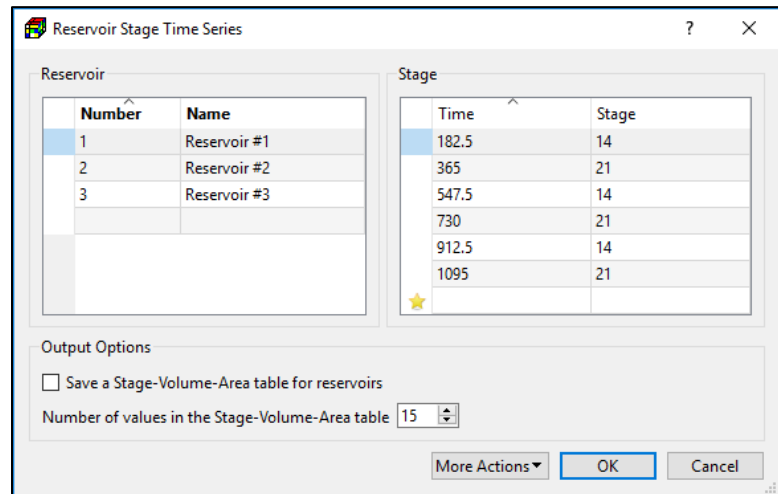
Figure 66. The Reservoir Stage Time Series dialog box

time and the corresponding stage to the Stage table. The observation time is expressed in the model time unit and is measured from the start of the model simulation. The Reservoir package requires the input of the starting and ending stages for each stress period. The stage values for each stress period are obtained by linear interpolation using the values specified in the Stage table. If the starting time of a stress period is earlier than the earliest observation time in the table, the earliest observed stage is used as the starting stage for that stress period. Similarly, if the end time of a stress period is beyond the latest observation time, the latest observed stage is used.

  - **Output Option**

    - Save a Stage-Volume-Area table for reservoirs: If this option is checked, reservoir stage, area, and volume (at the end of each time step) will be printed to the Run Listing File of MODFLOW.

    - Number of values in the stage-volume-area table: This is the number of values used to print the Stage-Volume-Area table. First and last stage value are

minimum and maximum elevations within area of potential inundation. A value of 15 or greater is recommended for detailed representation of stage-volume and stage-area relations.

3.8.1.1.14. Stream (STR)

The Stream (STR) Package (Prudic, 1989) is designed to account for flow in streams and to simulate the interaction between streams and groundwater. This package was originally called the Stream-flow Routing package and is renamed to the Stream Package in MODFLOW-2005 to avoid the naming conflict with the Streamflow-Routing (SFR1) Package[34] (Prudic, et al., 2004) and the SFR2 Package (Niswonger, et al., 2006). The STR, SFR1, and SFR2 packages should not be used in a model at the same time.

The STR Package is not a true surface water flow model, but rather is a bookkeeping program that tracks the flow in one or more streams which interact with groundwater. The STR Package limits the amount of groundwater recharge to the available streamflow. It permits two or more streams to merge into one with flow in the merged stream equal to the sum of the tributary flows. The STR Package also permits diversions from streams. The groundwater flow model with the STR Package has an advantage over the analytical solution in simulating the interaction between aquifer and stream because it can be used to simulate complex systems that cannot be readily solved analytically. The STR Package does not include a time function for streamflow but rather streamflow entering the modeled area is assumed to be instantly available to downstream reaches during each stress period. This assumption is generally reasonable because of the relatively slow rate of groundwater flow. Another assumption is that leakage between streams and aquifers is instantaneous. This assumption may not be reasonable if the streams and aquifers are separated by a thick unsaturated zone.

The STR Package divides streams into segments and reaches. Each reach corresponds to a model cell. A segment consists of a group of reaches connected in downstream order. Streamflow is accounted for by specifying flow for the first reach in each segment, and then computing stream-flow to adjacent downstream reaches in each segment as inflow in the upstream reach plus or minus leakage from or to the aquifer in the upstream reach. Streamflow into a segment that is formed from tributary streams is computed by adding the outflows from the last reach in each of the specified tributary segments. If a segment is a diversion, then the specified flow into the first reach of the segment is subtracted from flow in the main stream. However, if the specified flow of the diversion is greater than the flow out of the segment from which flow is to be diverted then no flow is diverted from that segment.

Multiple reach instances may be assigned to a model cell. For each reach, the flow rate Q_{str} [L³T⁻¹] between the reach and the model cell is calculated by the following equations.

---

[34] SFR1 is not supported by PM

$$Q_{str} = C_{str} \cdot (h_{str} - h) \qquad if\ h > B_{str}$$ (26)

$$Q_{str} = C_{str} \cdot (h_{str} - B_{str}) \quad if\ h \leq B_{str}$$ (27)

where

Q_{str} [L^{3}T^{-1}] is the flow rate between the reach and the model cell (i.e., the groundwater system). A positive value means that water flows from the reach to aquifer,

C_{str} [L^{2}T^{-1}] is the stream conductance.

h [L] is the calculated hydraulic head in the cell containing the reach,

h_{str} [L] is the stream stage (i.e., hydraulic head in the reach), and

B_{str} [L] is the elevation of the bottom of streambed sediments.

The cell-by-cell or polyline input methods may be used to specify the following stream data. The polygon input method is not supported. The polyline input method is recommended as it can assign the reach numbers in the required sequential order automatically.

1. **Cell-by-cell input method:** Figure 67 shows the dialog box for specifying reach properties.

   - **Calculate Stream Stage in Reaches:** If checked, the stream stage in each reach is calculated based on Manning's formula under the assumption of a rectangular stream channel. This option applies to the entire STR package.

   - **Include Concentration Data in the SSM Package of MT3D/SEAWAT:** If this box is checked, the values entered to **Concentration (MT3D/SEAWAT) [ML^{-3}]** are used as source water concentration. If this box is not checked, the concentration of the source water is assumed to be zero.

   - **Segment (Cell Properties)**

Figure 67. The Stream Package dialog box for specifying cell properties

- o **Segment Number** [-]: The number of the segment to which the current reach belongs. Enter 0 to remove the cell from the segment.
- o **Inflow to this Segment [L^3T^{-1}]:** The streamflow entering the segment. Enter -1, if inflow into this segment is the sum of outflow from its tributary segments. If a segment is a diversion and the *Simulate diversions from segments box (see below)* is checked, then the specified inflow is subtracted from flow in the main stream. However, if the specified inflow of the diversion is greater than the flow out of the segment from which flow is to be diverted, then no flow is diverted from that segment.

- **Reach (Cell Properties):**
  - o **Reach Number [-]:** This is a sequential number in a segment that begins with one for the farthest upstream reach and continues in downstream order to the last reach in the segment.
  - o **Stream Stage (h_{str}) [L]** is the hydraulic head in the stream. Stream Stage is not used if "Calculate Stream Stage in Reaches" is checked.
  - o **Streambed Conductance (C_{str}) [L^2T^{-1}]:** The value describes the head loss between the stream and the aquifer. It depends on the material and characteristics of the streambed sediments and the immediate environment**.** The value of C_{str} can be estimated based on the following equation:

$$C_{str} = \frac{K_{str} \cdot L \cdot W_{str}}{T_{str} - B_{str}}$$
(28)

where

K_{str} [LT^{-1}] is the hydraulic conductivity of the streambed,

L [L] is the length of the stream reach within the cell,

W_{str} [L] is the width of the stream channel,

T_{str} [L] is the elevation of the top of the streambed sediments, and

B_{str} [L] is the elevation of the bottom of the streambed sediments.

  - o **Elevation of Streambed Top (T_{str}) [L]** is the elevation of the top of the streambed sediments.
  - o **Elevation of Streambed Bottom (B_{str}) [L]** is the elevation of the bottom of the streambed sediments.
  - o **Width of the Stream Channel (W_{str}) [L], Slope of the Stream Channel (S_{str}) [-], and Manning's Roughness Coefficient (n) [$TL^{-1/3}$]:** These parameters are used only when the box *Calculate Stream Stage in Reaches* is checked. To obtain the stream stage, the stream water depth (d_{str}) is calculated using the Manning's equation under the assumption of a rectangular stream channel. The calculated water

depth is added to T_{str} to get the stream stage. The Manning's equation for a stream channel is

$$Q = A \cdot R^{2/3} \cdot S_{str}^{1/2} / n \qquad (29)$$

where

Q [L³T⁻¹] is the calculated stream discharge,

A [L²] is the cross-sectional area of flow,

R [L] is the hydraulic radius, which is defined as A divided by the wetted perimeter,

S_{str} [-] is the slop of the stream channel, and

n [TL⁻¹ᐟ³]is the Manning's roughness coefficient.

The unit for Manning's roughness coefficient (n) is often left off, as n is usually given in SI units, for example [s/m$^{1/3}$]. If other units are used in the model, you should convert the value of n accordingly and enter the converted value to the model. For example, if your model uses [day] and [ft] for the time and length units, the following conversion applies

$$n = 1 \left[\frac{s}{m^{1/3}}\right] = \frac{1}{86400 \times 3.28^{1/3}} \left[\frac{day}{ft^{1/3}}\right] = \frac{1}{128383} \left[\frac{day}{ft^{1/3}}\right] \qquad (30)$$

Some conversion examples for other units are given below

$$n = 1 \left[\frac{s}{m^{1/3}}\right] = \frac{1}{86400} \left[\frac{day}{m^{1/3}}\right] = \frac{1}{1.486} \left[\frac{s}{ft^{1/3}}\right] \qquad (31)$$

o **Parameter Number (PEST) [-]** is used to group cells, where the C_{str} value is to be estimated by PEST. See *To define an estimable parameter* in Section 3.8.4 for details.

o **Concentration (MT3D/SEAWAT) [ML⁻³]:** Click the Edit button to open a Concentration dialog box (Figure 42) that allows you to specify the source water concentration of up to 100 species. The entered concentration values may be used by the SSM Package of MT3D or SEAWAT.

- **Structure:** Click this button to open the Stream Structure dialog box (Figure 68) that defines the structure of the stream system as shown in Figure 69. The table of dialog box indicates that segment 2 is diverted from segment 1, segment 1 is a tributary segment of segment 3, and segments 2 and 4 are tributary segments of segment 5.

Figure 68. The Stream Structure dialog box

o *Simulate diversions from segments*: Check this box to simulate diversions from segments.

o **Table:** Each row in the table represents a stream segment that is diverted from an upstream segment or has tributary segment(s).

  – **Segment #** is the number of the segment.

  – *Columns 1 to 10:* Each segment can have up to 10 tributary segments and their segment numbers are specified in the *respective columns.*

  – *Iupseg is* the number of the upstream segment from which water is diverted. For a segment that is not a diversion, *Iupseg* must be specified as zero. *Iupseg* is used only when the *Simulate diversions from segments* box is checked.
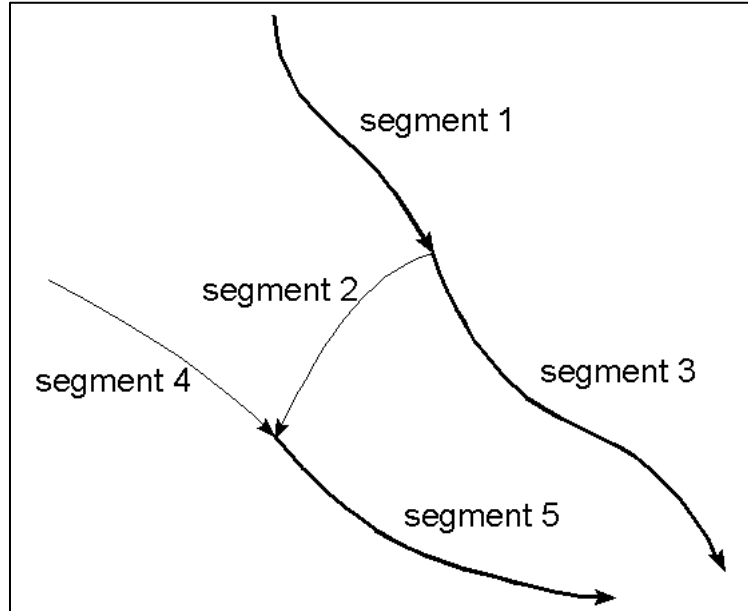
Figure 69. The stream system defined by the table in Figure 68

o **Add:** Click this button to add a row to the Table.

o **Delete:** Click this button to delete the selected row(s) from the Table.

2. **Polyline input method:** Figure 70 shows the dialog box for specifying vertex/polyline properties. Once the vertex data are specified, they may be interpolated and applied to model cells following the rules described in Section 3.3.2.2.

• **Simulation Settings:** Same as the cell-by-cell input method.

• **Segment (Polyline Properties)**

o **Auto Layer Number**

  – If this box is checked, the layer number of a stream reach alone the polyline is determined by comparing the elevation of the streambed bottom B_{str} of the reach with the top/bottom elevations of the cells in the same vertical model column as the reach.

    ▪ if B_{str} is higher than the top elevation of the highest cell, the reach is assigned to the cell in Layer 1.

- if B_{str} is lower than the bottom elevation of the lowest cell, the reach is assigned to the cell in Layer NLAY.
- If B_{str} lies between top and bottom elevations of a cell, the reach is assigned to that cell.

- If this box is not checked, the reaches along the polyline are assigned to the layer where the polyline is located.

o **Segment Number [-]:** The number of the segment to which the reaches along the polyline belong. Prior to applying a polyline to model cells, all existing reaches of the given segment number will be removed. Reach numbers will be assigned to the reaches along the polyline automatically.

o **Inflow to this Segment [L³T⁻¹]:** The streamflow entering the segment. Enter -1, if inflow into this segment is the sum of outflow from its tributary

Figure 70. The Stream Package dialog box for specifying vertex properties

segments. If a segment is a diversion, then the specified inflow is subtracted from flow in the main stream. However, if the specified inflow of the diversion is greater than the flow out of the segment from which flow is to be diverted, then no flow is diverted from that segment.

- **Reach (Vertex Properties):** The data of this group are assigned to one or more vertices of a polyline. These vertex data may be interpolated to model cells following the rules described in Section 3.3.2.2 and the rules below.

o **Streambed Conductance per Unit Length [LT⁻¹]** is interpolated to the reaches along the polyline. For each of those reaches, the interpolated value C_{strl} is multiplied with the length of the reach within the cell to obtain the streambed conductance C_{str}:

$$C_{str} = C_{strl} \cdot L_c \tag{32}$$

where

C_{strl} is the streambed conductance per unit length at a given cell, and

L_c is the length of the reach within the cell.

- o **Concentration (MT3D/SEAWAT) [ML⁻³]:** Click the Edit button to open a Concentration dialog box (Figure 42) that allows you to specify the source water concentration of up to 100 species to current vertex. The entered concentration values may be used by the SSM Package of MT3D or SEAWAT.
- o **The other parameters:** See the description in the cell-by-cell input method above.

- **Structure:** Same as the cell-by-cell input method.

3.8.1.1.15. Streamflow-Routing (SFR2)

The SFR2[35] Package (Niswonger, et al., 2006) is used to simulate streams in a model and is an alternative to the Stream (STR) Package, with the most important difference being that stream depth is computed at the midpoint of each reach instead of at the beginning of each reach, as was done in the STR Package. This approach allows for the addition and subtraction of water from runoff, precipitation, and evapotranspiration within each reach. The STR, SFR1[34], and SFR2 packages should not be used in a model at the same time.

In SFR2, the flow in a stream is either routed instantaneously to downstream streams or routed using a kinematic wave equation. Unsaturated flow is simulated independently of saturated flow within each model cell corresponding to a stream reach whenever the water table (head in MODFLOW) is below the elevation of the streambed. The relation between unsaturated hydraulic conductivity and water content is defined by the Brooks-Corey function. Unsaturated flow variables specified in SFR2 include saturated and initial water contents; saturated vertical hydraulic conductivity; and the Brooks-Corey exponent. These variables are defined independently for each stream reach.

Like the STR Package, the SFR2 Package divides streams into segments and reaches. A segment consists of a group of reaches connected in downstream order. One or more reaches may be assigned to a model cell. The cell-by-cell or polyline input methods may be used to specify the stream data. The polygon input method is not supported. The polyline input method is recommended as it can assign the reach numbers in the required sequential order automatically. The required input parameters are listed below.

---

[35] MODFLOW-2005 will not work if the SFR2 Package is activated and the *SFR* box of Modflow Output Control (Section 3.8.1.3) is checked. If the SFT Package of MT3D-USGS is not used, uncheck the *SFR* box. If you need to use the SFT Package, the *SFR* box must be checked and you must use MODFLOW-NWT for the flow simulation by either setting the UPW package as the internal flow package (Section 3.4.6) or assigning the executable of MODFLOW-NWT to the path of MODFLOW-2005 in Preferences (Section 3.4.11).

1. **All input methods:** The data-entry dialog boxes of all input methods contain an Options tab (Figure 71) with the following common data.

    - **ISFROPT** controls whether vertical unsaturated flow beneath stream reaches is simulated. The following available options are self-explanatory.

        o **Do not simulate vertical unsaturated flow beneath streams (ISFROPT = 1)**
        o **Simulate vertical unsaturated flow beneath streams (ISFROPT = 3)**

    - **Include Concentration Data in the SSM Package of MT3D/SEAWAT:** This determines how the entered concentration data are used, See **_Concentration (MT3D/SEAWAT) [ML^{-3}]_** below for details.

    - **Transient Streamflow Routing (TRANSROUTE):** When this box is checked, streamflow will be routed using the kinematic-wave equation, see p. 68-69 of (Markstrom, et al., 2008) for details about the kinematic-wave approximation. The following parameters are used to control the behavior of transient streamflow routing:

Figure 71. The Options tab of the Streamflow-Routing Package (SFR2) dialog box

    o **Number of Sub Time Steps (NUMTIM):** NUMTIM is the number of sub time steps used to route streamflow. The time step that will be used to route streamflow will be equal to the MODFLOW time step divided by NUMTIM.
    o **Time Weighting factor (WEIGHT):** This is used to calculate the change in channel storage. WEIGHT should have a value between 0.5 and 1. See equation 83 in (Markstrom, et al., 2008) for further details.
    o **Streamflow Tolerance (FLWTOL):** This is used for convergence of the kinematic wave equation. A value of 0.00003 m^3/s has been used successfully in test simulations of the SFR2 Package.

    - **Unsaturated Flow Options:** This group is activated only if ISFROPT is set to 3.

- o **Number of trailing wave increments (NSTRAIL):** This is the number of trailing wave increments used to represent a trailing wave. Trailing waves are used to represent a decrease in the surface infiltration rate. The value can be increased to improve mass balance in the unsaturated zone. As indicated by (Niswonger, et al., 2006), a value between 10 and 20 works well and results in unsaturated-zone mass balance errors beneath streams ranging between 0.001 and 0.01 percent.
- o **Maximum number of vertical cells for the unsaturated zone (ISUZN):** This is the maximum number of vertical cells used to the define the unsaturated zone beneath a stream reach. If ICALC is 1 for all segments then ISUZN should be set to 1 as suggested by (Niswonger, et al., 2006).
- o **Maximum number of different sets of trailing waves (NSFRSETS):** This is the maximum number of different sets of trailing waves used to allocate arrays. Arrays are allocated by multiplying NSTRAIL by NSFRSETS. A value of 30 is usually sufficient for problems where the stream depth varies often. However, in some cases a value of 50 may be required. If this value is set too small, then the simulation will terminate prematurely, and an error will be printed to the Run Listing file.

2. **Cell-by-cell input method:** Figure 72 shows the Properties tab of the Streamflow-Routing Package (SFR2) dialog box. The required data are organized in two groups as described below.

- **Time-Independent Reach Properties:** The following parameters remain unchanged for the entire simulation.
  - o **Segment Number (ISEG) [-]:** The number of the segment to which the current cell belongs. Enter 0 to remove the cell from the segment.
  - o **Reach Number (IREACH) [-]:** Each model cell in a segment is a reach. IREACH is a sequential number in a segment that begins with one for the farthest
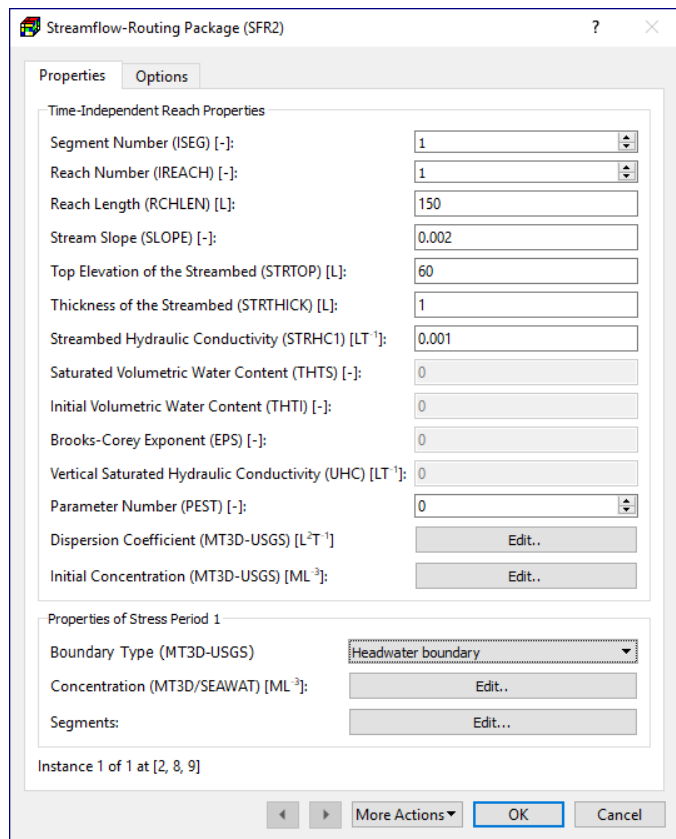
Figure 72. The Streamflow-Routing Package (SFR2) dialog box for specifying cell properties

upstream reach and continues in downstream order to the last reach in the segment.

o **Reach Length (RCHLEN) [L]:** Length of the stream reach within the model cell.

o **Stream Slope (SLOPE) [-]**: Stream slope across the reach.

o **Top Elevation of the Streambed (STRTOP) [L]:** Average elevation of the top of the streambed within model cell.

o **Thickness of the Streambed (STRTHICK) [L]:** Average thickness of the streambed within the model cell.

o **Streambed Hydraulic Conductivity (STRHC1) [LT^{-1}]:** Average hydraulic conductivity of the streambed within the model cell.

o **Saturated Volumetric Water Content (THTS) [-]:** Value of the saturated volumetric water content in the unsaturated zone beneath the stream reach.

o **Initial Volumetric Water Content (THTI) [-]:** Initial value of the volumetric water content in the unsaturated zone beneath the stream reach. The value of THTI must meet this requirement: THTS – Sy ≤ THTI ≤ THTS.

o **Brooks-Corey Exponent (EPS) [-]:** The Brooks-Corey exponent is used in the relation between water content and hydraulic conductivity within the unsaturated zone.

o **Vertical Saturated Hydraulic Conductivity (UHC) [LT^{-1}]:** Vertical saturated hydraulic conductivity of the unsaturated zone beneath the stream reach.

o **Parameter Number (PEST) [-]** is used to group cells, where the STRHC1 is to be estimated by PEST. See *To define an estimable parameter* in Section 3.8.4 for details.

o **Observation Point [-]:** If this box is checked, the Streamflow Transport (SFT) package of MT3D-USGS will write the simulated concentration to the Streamflow Transport Package Observation file (mt3d.sft.obs).

o **Dispersion Coefficient (MT3D-USGS) [L^{2}T^{-1}]:** Click the Edit button to specify stream dispersion coefficient associated with the current reach. The stream dispersion coefficient can vary for each species. The specified values are used by the Streamflow Transport (SFT) package of MT3D-USGS.

o **Initial Concentration (MT3D-USGS) [ML^{-3}]:** Click the Edit button to specify initial stream constituent concentration associated with the current reach. The specified values are used by the Streamflow Transport (SFT) package of MT3D-USGS.

- **Properties for Current Stress Period:** The following properties will be used for the current stress period.

o **Boundary Type (MT3D-USGS):** This defines the boundary condition (ISFBCTYP) of the current reach in the SFT Package.

  – **Headwater boundary.** That is for streams entering at the boundary of the simulated domain that need a specified concentration

- **Precipitation boundary.** Use this option if precipitation (i.e., PPTSW in Figure 73) directly to channels is simulated in the flow model and a non-zero concentration (default is zero) is desired.
- **Runoff boundary.** Use this option if you want to assign a non-zero concentration (default is zero) associated with the runoff values (i.e., RUNOFF in Figure 73).
- **Constant-concentration boundary.** Any reach number may be set equal to a constant concentration boundary condition.

o **Concentration (MT3D/SEAWAT) [ML^{-3}]:** Click the Edit button to open a Concentration dialog box (Figure 42) that allows you to specify the concentration of up to 100 species to the current reach. The specified concentration data will be used in the following manner:

- If MT3D-USGS is the selected Transport Model (Figure 96) and its SFT Package is activated, the concentration data will be associated with the specified Boundary Type in the SFT Package. The concentration data will not be used in the SSM Package.
- If the selected Transport Model is MT3DMS or SEAWAT, and the *Include Concentration Data in the SSM Package of MT3D/SEAWAT* box is checked, the concentration data will be used as specified concentration of the stream water in the SSM Package.
- If neither of the cases applies, the concentration data will not be used.

o **Segments:** Click the Edit button to open the SFR2 Segments dialog box (Figure 73). This dialog box contains a table and several buttons as described flow. Each row of the table in this dialog box represents a segment of the current stress period.

- **Add**: Click this button to add a row to the table.
- **Delete:** Click this button to delete the selected row(s) from the table.
- **X-Section:** Click this button to open the *Eight-point Cross Section* dialog box that allows you to edit the 8-point channel cross-section of the selected row. If more than one rows are selected, the data of the row with the smallest segment number will be edited. The *Eight-point Cross Section* dialog box contains a table with two columns – XCPT and ZCPT. XCPT is the distance

SFR2 Segments ? ✕

Properties of Stress Period 1

NSEG	ICALC	OUTSEG	IUPSEG	IPRIOR	FLOW	RUNOFF	ETSW	PPTSW	ROUGHCH	ROUGHBK	WIDTH1	WIDTH2	DEPTH1	DEPTH2
1	0	0	0	0	0.01	0	0	0	0	0	100	100	50	50
2	2	0	0	0	0	0	0	0	1e-5	1e-6	0	0	0	0

[Add] [Delete] [X-Section] [More Actions ▼] [OK] [Cancel]
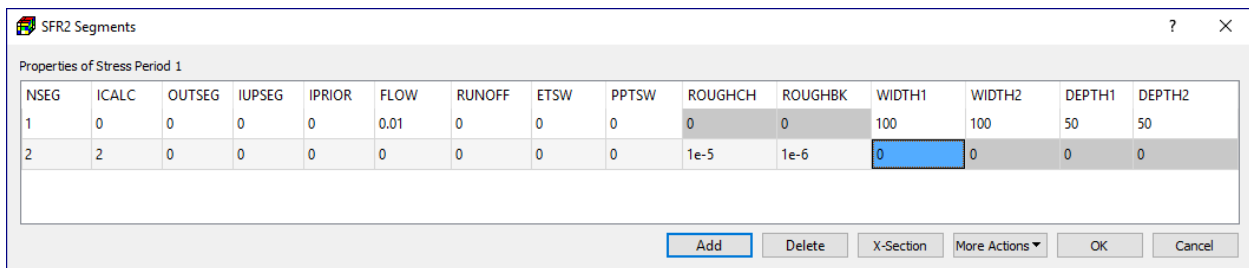
Figure 73. The SFR2 Segments dialog box

relative to the left bank of the stream channel (when looking downstream) for the eight points used to describe the geometry of the segment of the stream channel. ZCPT is the height relative to the top of the lowest elevation of the streambed. The lowest elevation (ZCPT = 0.0) can be any one from Point 2 through 7.

- **More Actions**: Use the functions of this dropdown menu to save the table contents to a file; or to load the table contents from a file.
- **Table:** A cell in the table is greyed out, if its data will not be used. The columns of the table are described below.

  - **NSEG**: Segment number
  - **ICALC** is a flag that controls the calculation of stream depth:

    - ICALC = 0: Stream depth is specified by DEPTH1 and DEPTH2 at the beginning of a stress period and remains unchanged unless flow at the midpoint of a reach is zero, then depth is set to zero in that reach. No unsaturated flow is allowed.
    - ICALC = 1: Stream depth is calculated using Manning's equation and assuming a wide rectangular channel. Unsaturated flow is simulated when ISFROPT > 1 and the value of ICALC must remain 1 for the specified segment during the simulation.
    - ICALC = 2: Stream depth is calculated using Manning's equation and assuming an eight-point channel cross section for each segment (which allows for the computation of a wetted perimeter and for changing hydraulic conductance of the streambed in relation to changes in flow). Unsaturated flow is simulated when ISFROPT > 1 and the value of ICALC must remain 2 for the specified segment during the simulation.

  - **OUTSEG** is the segment number of the downstream segment that receives tributary inflow from the last reach of this segment. If the segment ends within the modeled grid and OUTSEG = 0, outflow from the segment is not routed anywhere and is no longer part of the stream network. One may wish to use this if all flow in the stream gets diverted into a lined canal or into a pipe. If the flow out of this segment discharges into a lake, set OUTSEG equal to the negative value of the lake identification number
  - **IUPSEG** is the number of the upstream segment from which water is diverted (or withdrawn) to supply inflow to this segment. If the source of a stream segment is discharge from a lake, set IUPSEG equal to the negative value of the lake identification number. If this stream segment does not receive inflow from a lake or as a diversion from an upstream segment, set IUPSEG to zero.

- **IPRIOR** defines the prioritization system for diversion and is used in conjunction with the value of FLOW (see below). IPRIOR is used only if IUPSEG > 0.
- **FLOW** [L^3/T]**:** If the segment is a head water stream, FLOW is the streamflow entering the first reach of the segment. If the segment is a tributary stream, FLOW is the flow added to or removed from the first reach of the segment. If the segment is a diversionary stream (i.e., IUPSEG is not 0), FLOW and IPRIOR are used together to define the flow (Qd) that may be diverted from IUPSEG to this segment.

  - IPRIOR = 0: Qd = min(FLOW, Q)
  - IPRIOR = -1: Qd = 0 if FLOW > Q otherwise Qd = FLOW.
  - IPRIOR = -2: Qd = FLOW x Q, in this case 0.0 ≤ FLOW ≤ 1.0
  - IPRIOR = -3: Qd = Q if FLOW > Q otherwise Qd = 0

   where Q is flow available in the IUPSEG segment.
- **RUNOFF** [L^3/T] is the volumetric rate of the diffuse overland runoff that enters the stream segment.
- **ETSW** [L/T] is the volumetric rate per unit area of water removed by evapotranspiration directly from the stream channel. ETSW is defined as a positive value.
- **PPTSW** [L/T] is the volumetric rate per unit area of water added by precipitation directly on the stream channel.
- **ROUGHCH** is Manning's roughness coefficient for all reaches in this segment. See Section 3.8.1.1.14 for a discussion of Manning's roughness coefficient.
- **ROUGHBK** is Manning's roughness coefficient for the overbank area in all reaches in this segment. This value is used only if ICALC = 2.
- **WIDTH1** [L] is the width of the stream channel at the upstream end of this segment.
- **WIDTH2** [L] is the width of the stream channel at the downstream end of this segment.
- **DEPTH1** [L] is the depth of water in the stream channel at the upstream end of this segment.
- **DEPTH2** [L] is the depth of water in the stream channel at the downstream end of this segment.

3. **Polyline input method:** Figure 74 shows the Properties tab of the Streamflow-Routing Package (SFR2) dialog box. The required data are organized in two groups as described below. Once the vertex data are specified, they may be interpolated and applied to model cells following the rules described in Section 3.3.2.2.

- **Time-Independent Reach Properties**

  o **Layer Number**

    - Current Layer: Assign cells along the polyline to the current layer.
    - Highest Active Layer: Assign the cells along the polyline to the highest active layer.
    - Streambed Elevation: Assign the cells along the polyline to a layer where the elevation of the streambed bottom (STRTOP - STRTHICK) lies between the layer's upper and lower bounds. A cell is set to the highest/lowest layer, if (STRTOP - STRTHICK) is higher/lower than the model top/bottom.
    - Highest Active Layer & Streambed Elevation: Assign the cells along the polyline to the highest active layer where the elevation of the streambed bottom lies between the layer's upper and lower bounds. If the streambed bottom of a cell does not lie within a layer's lower and upper bounds, the cell is assigned to the highest active layer.

Figure 74. The Streamflow-Routing Package (SFR2) dialog box for specifying vertex properties

  o **Segment Number (ISEG) [-]:** The number of the segment to which the reaches along the polyline belong. Prior to applying a polyline to model cells, all existing reaches of the given segment number will be removed. Reach numbers will be assigned to the reaches along the polyline automatically.

  o **Reach (Vertex Properties):** See cell-by-cell input method above for the description of the parameters in this group.

- **Properties for Current Stress Period:** The following properties will be used for the current stress period.

- o **Concentration (MT3D/SEAWAT) [ML⁻³]:** Click the Edit button to open a Concentration dialog box (Figure 42) that allows you to specify the concentration of up to 100 species to the current vertex. Depending on the selected Concentration option in the Option tab, the entered values may be used as the source water concentration in the SSM package or the specified concentration of the selected boundary type in the SFT package.
- o **Segments:** Same as the cell-by-cell input method above.

3.8.1.1.16. Subsidence and Aquifer-System Compaction (SUB)

The SUB Package (Hoffmann, et al., 2003) simulates elastic (recoverable) compaction and expansion, and inelastic (permanent) compaction of compressible fine-grained beds (interbeds) within the aquifers. The deformation of the interbeds is caused by head or pore-pressure changes, and thus by changes in effective stress, within the interbeds. If the stress is less than the preconsolidation stress of the sediments, the deformation is elastic; if the stress is greater than the preconsolidation stress, the deformation is inelastic. The propagation of head changes within the interbeds is defined by a transient, one-dimensional (vertical) diffusion equation. This equation accounts for delayed release of water from storage or uptake of water into storage in the interbeds. Properties that control the timing of the storage changes are vertical hydraulic diffusivity and interbed thickness. The SUB Package supersedes the IBS Package (Section 3.8.1.1.8), which assumes that water is released from or taken into storage with changes in head in the aquifer within a single model time step and, therefore, can be reasonably used to simulate only thin interbeds. The SUB Package relaxes this assumption and can be used to simulate time-dependent drainage and compaction of thick interbeds and confining units. The time-dependent drainage can be turned off, in which case the SUB Package gives results identical to those from IBS.

The required input parameters for the cell-by-cell input methods are listed below. The polyline and polygon input methods are not supported.

1. **Cell-by-cell input method:** Figure 75 shows the dialog box for specifying cell properties.
   - **Data Tab**
     - o **No-delay Interbeds**
       - – **Number of Interbeds (NNDB) [-]:** This is the number of the systems of no-delay interbeds.
       - – **Layer Assignment (LN):** Click the Edit button to open the Layer Assignment dialog box that allows you to assign systems no-delay interbeds to model layers.
       - – **Properties of Interbed Systems:** the following values need to be assigned to each system of no-delay interbeds:
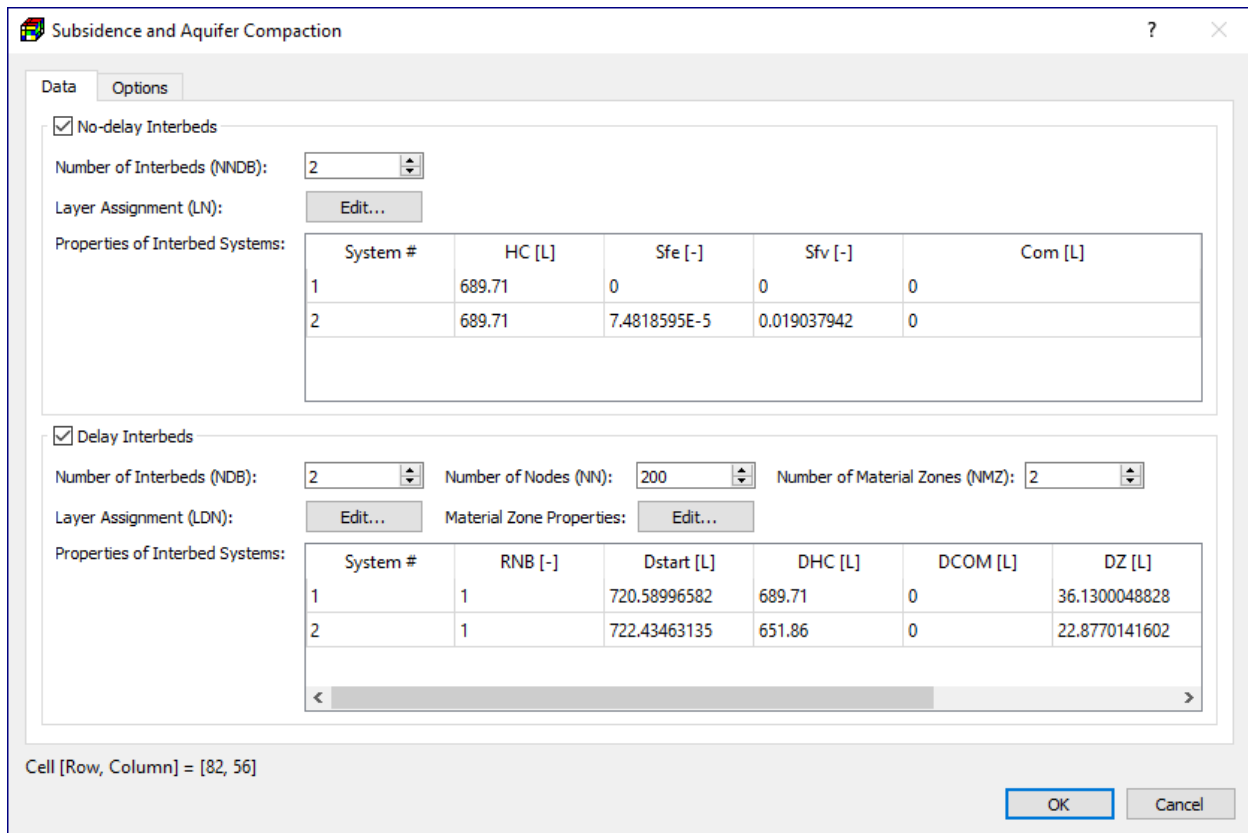
Figure 75. The Subsidence and Aquifer Compaction dialog box

- **HC [L]:** this is the preconsolidation head. For any model cells in which the specified HC is greater than the starting hydraulic head, the value of the starting head will be used in the simulation instead of HC.
- **Sfe [-]:** this is the dimensionless elastic skeletal storage coefficient.
- **Sfv [-]:** this is the dimensionless inelastic skeletal storage coefficient.
- **Com [L]:** this is the starting compaction. The value of *Com* does not affect the calculation. It is merely added to the computed compaction value so that the stored result values of compaction and subsidence may include previous components defined by *Com*.

o **Delay Interbeds**

- **Number of Interbeds (NDB):** This is the number of the systems of delay interbeds. To reduce the number of computations required, delay interbeds with the same vertical hydraulic conductivity and elastic and inelastic skeletal specific storage within one model layer can be grouped into one system of delay interbeds.
- **Number of Nodes (NN):** This is used to discretize the half of the equivalent thickness (DZ) of a system of delay interbeds to approximate the head distributions within the system of delay interbeds.

- **Number of Material Zones (NMZ):** NMZ is the number of material zones that are needed to define the hydraulic properties of systems of delay interbeds. Each material zone is defined by a combination of vertical hydraulic conductivity [LT^{-1}], elastic skeletal specific storage [L^{-1}], and inelastic skeletal specific storage [L^{-1}].
- **Layer Assignment (LDN):** Click the Edit button to open the Layer Assignment dialog box that allows you to assign systems delay interbeds to model layers.
- **Material Zone Properties:** Click the Edit button to open the Material Zone Properties dialog box that allows you to assign vertical hydraulic conductivity [LT^{-1}], elastic skeletal specific storage[L^{-1}], and inelastic skeletal specific storage [L^{-1}] to each material zone.
- **Properties of Interbed Systems:** the following values need to be assigned to each system of delay interbeds:

  - **RNB [-]** specifies the factor n_{equiv} for the systems of delay interbeds. See eq. 20 of (Hoffmann, et al., 2003) for details. RNB is also used to define the areal extent of each system of interbeds. For cells beyond the areal extent of the system of interbeds, enter a number less than 1.0.
  - **Dstart [L]** is the starting head values in systems of delay interbeds.
  - **DHC [L]** is the starting preconsolidation head for systems of delay interbeds. For any model cells in which the specified DHC is greater than the starting hydraulic head, the value of the starting head will be used in the simulation instead of HC.
  - **DCOM [L]** is the starting compaction in systems of delay interbeds. The value of *DCOM* does not affect the calculation. It is merely added to the computed compaction value so that the stored result values of compaction and subsidence may include previous components defined by *DCOM*.
  - **DZ [L]** is the equivalent thickness of systems of delay interbeds. See eq. 19 of (Hoffmann, et al., 2003) for details.
  - **NZ [-]** is the zone number for systems of delay interbeds. The zone number and the Material Zone Properties define the vertical hydraulic conductivity, elastic skeletal specific storage, and inelastic skeletal specific storage at the cell location.

- **Options Tab (**Figure 76**)**

  o **Solver**

  - **Acceleration Parameter (AC1):** This is ω1 in equation 25 of (Hoffmann, et al., 2003). It is used to predict the aquifer head at the interbed boundaries based on the head change computed for the previous iteration. A value of 0.0 results in the use of the aquifer head at the previous iteration. Limited experience indicates that optimum values may range from 0.0 to 0.6.
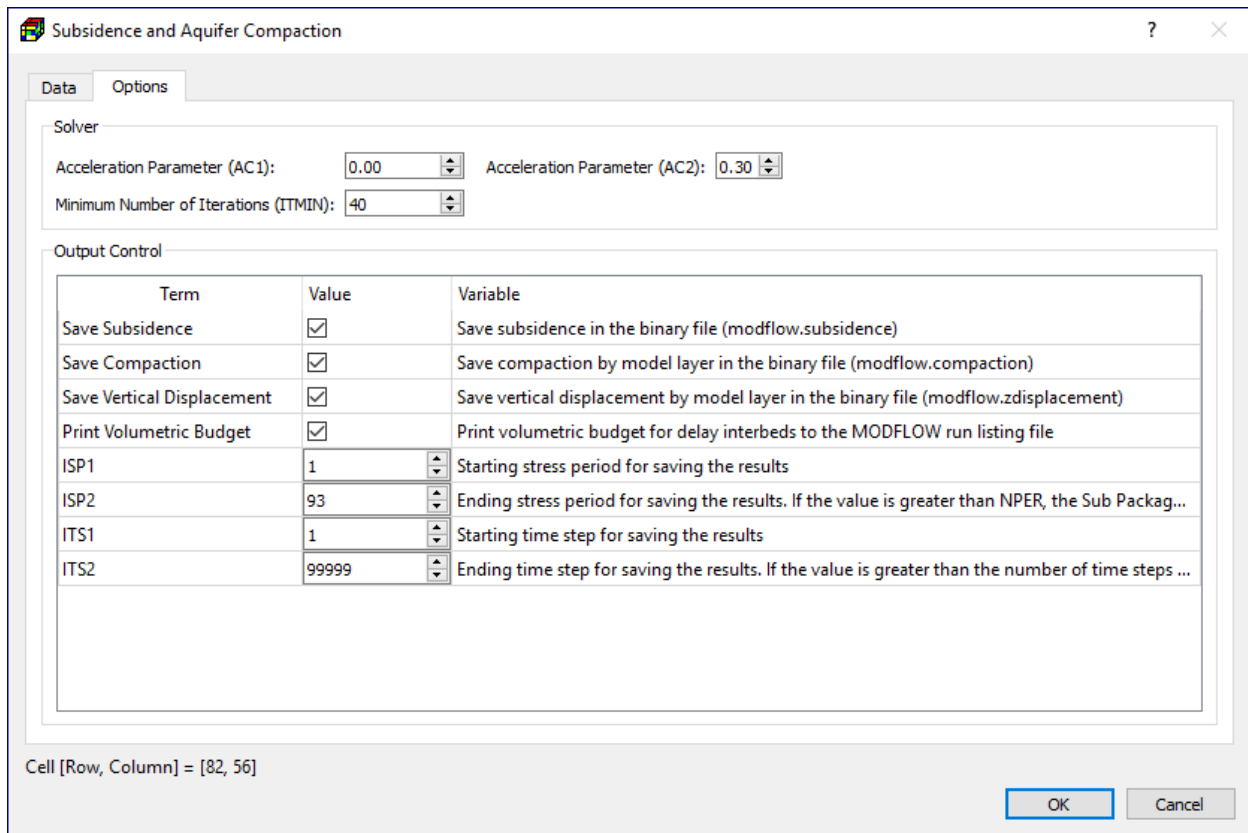
Figure 76. The Options tab of the Subsidence and Aquifer Compaction dialog box

- **Acceleration Parameter (AC2):** This is ω2 in equation 27 of (Hoffmann, et al., 2003). It is a multiplier for the head changes to compute the head at the new iteration. Values are normally between 1.0 and 2.0. This parameter also can be used to help convergence of the iterative solution by using values between 0 and 1.

- **Minimum Number of Iterations (ITMIN):** This is the minimum number of iterations for which one-dimensional equations will be solved for flow in interbeds when the Strongly Implicit Procedure (SIP) is used to solve the ground-water flow equations. If the current iteration level is greater than ITMIN and the SIP convergence criterion for head closure (HCLOSE) is met at a cell, the one-dimensional equations for that cell will not be solved. The previous solution will be used. The value of ITMIN is not used if a solver other than SIP is used to solve the ground-water flow equations.

o **Output Control**

- **Save Subsidence:** Check this box to instruct the SUB Package to save subsidence in the binary file modflow.subsidence. Subsidence is the sum of the compaction from all interbed systems, including no-delay and delay systems.

- **Save Compaction:** Check this box to instruct the SUB Package to save compaction by model layer in the binary file modflow.compaction. The SUB Package computes compaction for each system of interbeds. The model layer numbers to which each system belongs are specified in arrays LN and LDN for no-delay and delay systems, respectively. Each model layer can include more than one system of interbeds of either type or combinations of both types. The output option of compaction by model layer is the sum of compaction of all systems within each model layer.
- **Save Vertical Displacement:** Check this box to instruct the SUB Package to save vertical displacement by model layer in the binary file modflow.zdisplacement. Vertical displacement for a model layer is defined as the sum of the compaction in the layer and in all underlying layers. This displacement corresponds to movement of the upper surface of the model layer. The vertical displacement for layer 1 is equal to the subsidence. Any layers below the lowest system of compressible interbeds will have zero vertical displacement.
- **Print Volumetric Budget:** Check this box to instruct the SUB Package to print volumetric budget for delayed interbeds to the MODFLOW run listing file.
- **ISP1** is the starting stress period for saving the results.
- **ISP2** is the ending stress period for saving the results. If the value is greater than NPER, the Sub Package will change it to NPER.
- **ITS1** is the starting time step for saving the results.
- **ITS2** is the ending time step for saving the results. If the value is greater than the number of time steps in a given stress period, the Sub Package will change it to the number of time steps in that stress period.

3.8.1.1.17. Seawater Intrusion 2 (SWI2)

The SWI2 Package (Bakker, et al., 2013) allows three-dimensional vertically integrated variable-density groundwater flow and seawater intrusion in coastal multi-aquifer systems to be simulated using MODFLOW-2005. The main advantage of the formulation used in the SWI2 Package compared to models that solve flow and transport equations is that the SWI2 Package represents three-dimensional vertically integrated variable-density flow without the need to discretize the aquifer vertically. Vertically integrated variable-density groundwater flow is based on the Dupuit approximation in which an aquifer is vertically discretized into zones of differing densities, separated from each other by defined surfaces representing interfaces or density isosurfaces. The numerical approach used in the SWI2 Package does not account for diffusion and dispersion and should not be used where these processes are important. The resulting differential equations are equivalent in form to the groundwater flow equation for uniform-density flow. The approach implemented in the SWI2 Package allows density effects to be incorporated into MODFLOW-2005 through the addition of pseudo-source terms to the groundwater flow equation without the need to solve a separate advective-dispersive transport equation. Vertical and horizontal movement of defined density surfaces is calculated separately

using a combination of fluxes calculated through solution of the groundwater flow equation and a simple tip and toe tracking algorithm.

The required input parameters for all input methods are identical and listed below.

1. **All input methods:**
   - **Data Tab (**Figure 77**)**
     - **Number of ZETA Surfaces (NSRF) [-]:** This is the number of active surfaces (i.e., interfaces between zones).
     - **Toe Slope (TOESLOPE) [-]:** Maximum slope of toe cells
     - **Tip Slope (TIPSLOPE) [-]:** Maximum slope of tip cells
     - **ALPHA [-]:** Fraction of threshold used to move the tip and toe to adjacent empty cells when the slope exceeds user-specified TOESLOPE and TIPSLOPE values. ALPHA must be greater than 0.0 and less than or equal to 1.0.
     - **BETA [-]:** Fraction of threshold used to move the toe to adjacent non-empty cells when the surface is below a minimum value defined by the user-specified TOESLOPE value. BETA must be greater than 0.0 and less than or equal to 1.0.
     - **Density Distribution Option (ISTRAT) [-]:** This is a flag indicating density distribution.
     - **Dimensionless Density (NU) [-]:** The dimensionless density v is defined as $v = (\rho - \rho_f)/\rho_f$, where ρ is the fluid density [M/L^3], and ρ_f is the density of freshwater [M/L^3]. Click the Edit button to specify the NU values in a Density dialog box.
       - If ISTRAT is *"density varies linear between surfaces"*, NSRF + 1 density values are to be specified. Each value represents the density of the corresponding zone.
       - If ISTRAT is *"density is constant between surfaces"*, NSRF + 2 density values are to be specified. The first value is the density along the top of highest zone (i.e.,
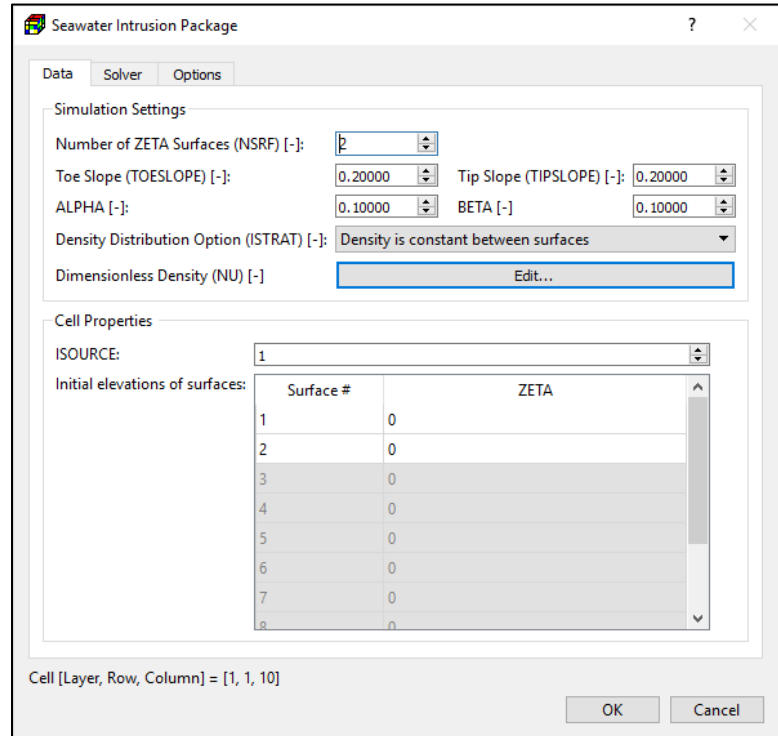
Figure 77. The Data tab of the Seawater Intrusion Package dialog box

first zone), followed by density values along each interface, and the density value at the bottom of the lowest zone (i.e. last zone).

o **ISOURCE**: Source type of any external sources or sinks, specified with any outside package (i.e., WEL, RCH, or GHB Package). There are three options:

- If ISOURCE > 0: Sources and sinks have the same fluid density as the zone ISOURCE. If such a zone is not present in the cell, sources and sinks have the same fluid density as the active zone at the top of the aquifer.
- If ISOURCE = 0: Sources and sinks have the same fluid density as the active zone at the top of the aquifer.
- If ISOURCE < 0: Sources have the same fluid density as the zone with a number equal to the absolute value of ISOURCE. Sinks have the same fluid density as the active zone at the top of the aquifer. This option is useful for the modeling of the ocean bottom where infiltrating water is salt, yet exfiltrating water is of the same type as the water at the top of the aquifer.

o **Initial Elevations of Surfaces:** Use the table to specify the initial elevations of the ZETA surfaces (i.e., interface between zones).

- An elevation for each surface needs to be specified for every cell in the model, even though a zeta surface is two-dimensional in most cases.
- When the specified Zeta surface value is above the top of the model layer, SWI2 requires the Zeta surface value to be set to the top of model layer in its input file, similarly when the specified Zeta surface value is below the bottom of model layer, SWI2 requires the Zeta surface value to be set to the bottom of model layer. PM will automatically adjust the Zeta surface based on this requirement when creating the input file for SWI2. Therefore, if a surface is present at only one point in the vertical everywhere, the same grid of ZETA values may be entered for every model layer.
- It is important to start with a reasonably smooth variation of the ZETA surface because it is not physically reasonable for a surface to be discontinuous or have sharp changes in gradient. When an irregular ZETA surface is entered, additional time in a transient simulation may be required before a physically realistic ZETA elevation is achieved in each cell, and it may take small time steps to reach an accurate solution.

• **Solver Tab (**Figure 78**)**

o **Solver (NSOLVER) [-]:** The solver used to solve for ZETA surfaces.
o **Printout Option (MUTSOL):** This controls printing of convergence information from the solver.
o **Printout Interval (IRPSOL):** The extreme head change and residual (positive or negative) 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 value of the printout interval.

o **NPCOND**: This is the matrix preconditioning method.

o **NBPOL**: This is used with the Neuman series polynomial preconditioning method. Checking this box to calculate the estimate of the
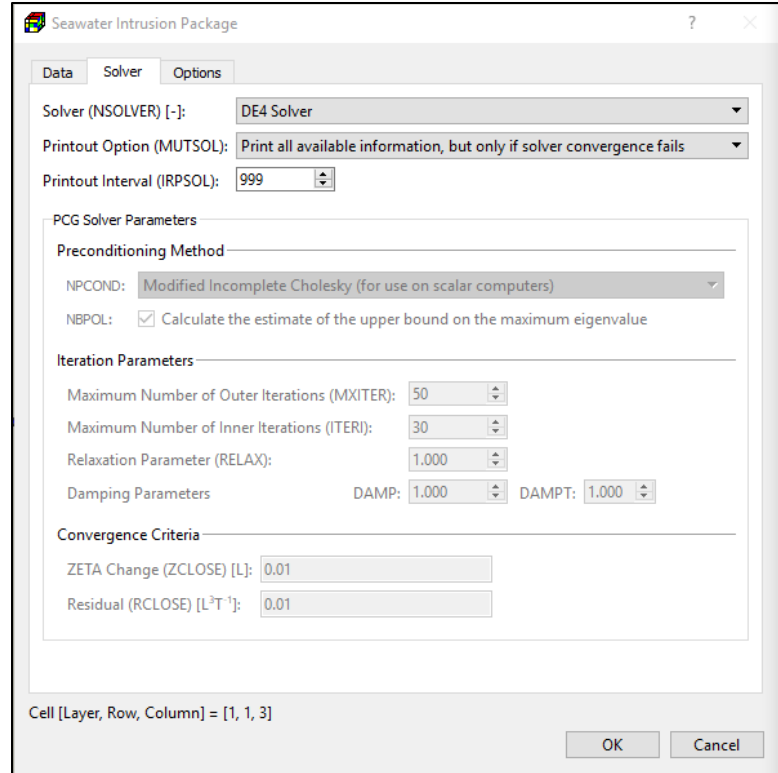
Figure 78. The Solver tab of the Seawater Intrusion Package dialog box

upper bound on the maximum eigenvalue. If this box is cleared, the estimate is set as 2. Convergence is generally insensitive to this parameter.

o **Maximum Number of Outer Iterations (MXITER):** For a linear problem MXITER should be 1, unless more than 50 inner iterations are required, when MXITER could be as large as 10. A larger number (generally less than 100) is required for a nonlinear problem.

o **Maximum Number of Inner Iterations (ITERI):** For nonlinear problems, ITERI usually ranges from 3 to 10; a value of 30 will be sufficient for most linear problems.

o **Relaxation Parameter (RELAX):** This is the relaxation parameter used with the Modified Incomplete Cholesky preconditioning method. Usually, RELAX=1.0, but for some problems a value of 0.99, 0.98, or 0.97 will reduce the number of iterations required for convergence.

o **Damping Parameters**

  − **DAMP**

    ▪ If DAMP > 0, it applies to both steady-state and transient stress periods.
    ▪ If DAMP < 0, it applies to steady-state periods. The absolute value is used as the damping factor.

- **DAMPT i**s the damping factor for transient stress periods and is only used when DAMP is specified as a negative value.
    - o **ZETA Change (ZCLOSE) [L]:** This is the ZETA change criterion for convergence. When the maximum absolute value of ZETA change from all nodes during an iteration is less than or equal to ZCLOSE, and the criterion for RCLOSE is also satisfied, iteration stops.
    - o **Residual (RCLOSE) [L³/T]:** This is the residual criterion for convergence. When the maximum absolute value of the residual at all nodes during an iteration is less than or equal to RCLOSE, and the criterion for ZCLOSE is also satisfied, iteration stops.

- **Options Tab**
    - o **Adaptive Time Stepping:** Check this box to enable adaptive time stepping algorithm that dynamically adjust the number of SWI2 time steps in a MODFLOW time step. The algorithm has no effect on the lengths of MODFLOW time steps and stress periods. Use of this option will increase the number of SWI2 time steps used during a MODFLOW time step when the tip or toe movement exceeds a user-defined value.
    - o **NADPTMX [-]:** Maximum number of SWI2 time steps per MODFLOW time step.
    - o **NADPTMN [-]:** Minimum number of SWI2 time steps per MODFLOW time step. NADPTMN must be less than or equal to NADPTMX.
    - o **ADPTFCT [-]:** ADPTFCT is the factor used to evaluate tip and toe thicknesses and control the number of SWI2 time steps per MODFLOW time step.

3.8.1.1.18. Time-Variant Specified Head (CHD)

For transient simulations, the Time-Variant Specified-Head (CHD) Package described in Appendix C of (Leake, et al., 1991) allows constant head cells to take on different head values for each time step. It provides a means of simulating head variations with time that can be approximated with piecewise linear segments. The CHD Package does not alter the way constant-head boundaries are formulated in MODFLOW.

The required input parameters for all input methods are identical and listed below.

1. **All input methods[36]:** Figure 79 shows the dialog box for specifying cell, vertex, or polygon properties.

    - **Flag [-]:** A non-zero value indicates that a cell is specified as a time-variant specified-head boundary.
        - o A no-flow cell cannot be converted to a CHD-cell.
        - o If a cell is specified as a time-variant specified-head boundary for a stress period and omitted in the specification for a subsequent period, it remains a constant-

---

[36] If multiple instances of CHD are assigned to a single cell, only one instance with the average values of h_s, h_e, and d of all instances will be use in the simulation.

head boundary with a head equal to the end head of the last stress period for which it was specified.

Figure 79. The Time-Variant Specified Head Package dialog box

- **Start Head (h_s) [L]**[36] and **End Head (h_e) [L]**[36]: These values are the prescribed hydraulic head of the cell at the start and end of a stress period, respectively. For each time step within the stress period, the prescribed hydraulic head h at the cell is determined by

$$h = h_s + (h_e - h_s) \cdot \frac{PERTIM}{PERLEN} \qquad (33)$$

where

$PERTIM$ is the starting time of the time step, and

$PERLEN$ is the length of the stress period.

The interpolated head values remain constant during the time step.

- **Head Conversion (SEAWAT):** This option determines how SEAWAT converts the specified values of h_s and h_e to reference head. Four options are available:

  o Use calculated water density at the cell
  o Use the specified water density value
  o Use the average of the calculated water density of the overlying cells
  o Input head values are reference head. No conversion

- **Water Density (d) [ML^{-3}] (SEAWAT)**[36]: Required only if the Head Conversion option is *Use the specified water density value.* SEAWAT uses this value to convert input head values to reference head.

3.8.1.1.19. Unsaturated-Zone Flow (UZF1)

The Unsaturated-Zone Flow (UZF1) Package (Niswonger, et al., 2006) was developed to simulate water flow and storage in the unsaturated zone and to partition flow into evapotranspiration and recharge. The package also accounts for land surface runoff to streams and lakes.

A kinematic wave approximation to Richards' equation is solved by the method of characteristics to simulate vertical unsaturated flow. The approach assumes that unsaturated flow occurs in response to gravity potential gradients only and ignores negative potential gradients; the approach further assumes uniform hydraulic properties in the unsaturated zone for each vertical column of model cells. The Brooks-Corey function is used to define the relation between

unsaturated hydraulic conductivity and water content. Residual water content is calculated internally by the UZF1 Package based on the difference between saturated water content and specific yield.

The UZF1 Package is a substitution for the Recharge and Evapotranspiration Packages. The UZF1 Package differs from the Recharge Package in that an infiltration rate is applied at land surface instead of a specified recharge rate directly to ground water. The applied infiltration rate is further limited by the saturated vertical hydraulic conductivity. The UZF1 Package differs from the Evapotranspiration Package in that evapotranspiration losses are first removed from the unsaturated zone above the evapotranspiration extinction depth, and if the demand is not met, water can be removed directly from ground water whenever the depth to ground water is less than the extinction depth. The UZF1 Package also differs from the Evapotranspiration Package in that water is discharged directly to land surface whenever the altitude of the water table exceeds land surface.

The required input parameters for all input methods are identical and listed below. Although these parameters are to be assigned to each vertical column of model cells, you may move between layers within the Data Editor to examine the grid configuration in each layer.

1. **All input methods:** Figure 80 shows the dialog box for specifying cell, vertex, or polygon properties.

   - **Data Tab**

     o **UZF Option (NUZTOP) [-]:** Since recharge or discharge is calculated for only one cell in each vertical column of model cells, three options are available for specifying the cell where recharge or discharge is applied to:

       – 1. Recharge to and discharge from only the top model layer. This option assumes land surface is defined as top of layer 1.
       – 2. Recharge to and discharge from the specified layer in variable IUZFBND. This option assumes land surface is defined as top of layer specified in IUZFBND.
       – 3. Recharge to and discharge from the highest active cell in each vertical column. Land surface is determined as top of layer specified in IUZFBND. A constant head node intercepts any recharge and prevents deeper percolation.

     o **Package Data (Time-Independent)**

       – **Aerial Extent (IUZFBND) [-]:** This value is used to define the aerial extent of the active model in which recharge and discharge will be simulated.

         ▪ If IUZFBND = 0, recharge and discharge will not be simulated. IUZFBND should be set to 0 in no-flow (inactive) cells and in constant head cells.
         ▪ If IUZFBND < 0, the calculated infiltration will be added as recharge directly to groundwater, and storage changes in the unsaturated zone will be neglected.
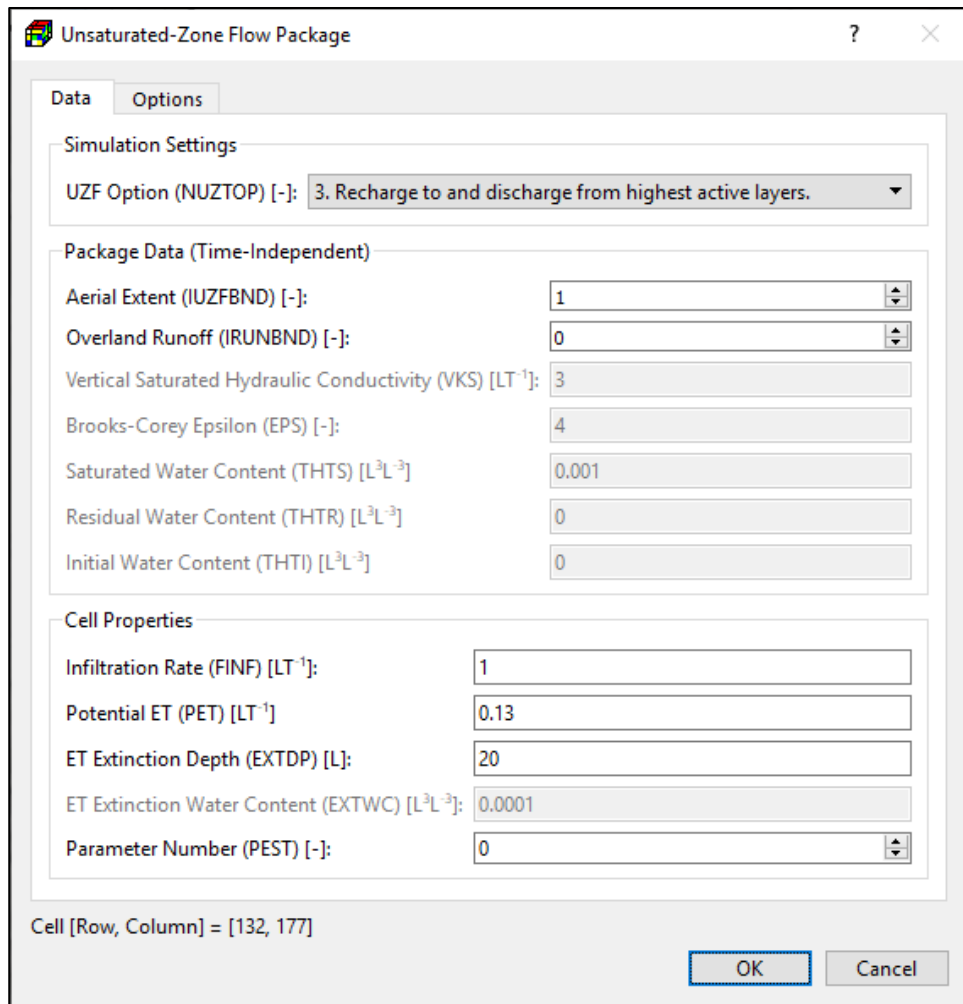
Figure 80. The Unsaturated-Zone Flow Package dialog box

- If NUZTOP = 2, the absolute value of IUZFBND indicates the layer where recharge and discharge occur.
- If NUZTOP ≥ 2, the absolute value of IUZFBND indicates the layer whose top is the land surface.

- **Overland Runoff (IRUNBND) [-]:** This value is used to define the stream segments within the Streamflow-Routing (SFR2) Package or lake numbers in the Lake (LAK3) Package to which overland runoff from excess infiltration and groundwater discharge to land surface will be added. A positive integer value identifies the stream segment and a negative integer value identifies the lake number.

- **Vertical Saturated Hydraulic Conductivity (VKS) [LT⁻¹]:** This is the vertical saturated hydraulic conductivity of the UZF cell. If VKS is the same as VK, you can use Tools > Data > Copy to copy VK to VKS.

- **Brooks-Corey Epsilon (EPS) [-]:** The epsilon exponent is used in the relation of water content to hydraulic conductivity.
- **Saturated Water Content (THTS) [$L^3 L^{-3}$]:** The saturated water content is approximately the same as the porosity.
- **Residual Water Content (THTR) [$L^3 L^{-3}$]:** the residual water content, commonly defined as the water content θ for which the gradient $d\theta/dh$ becomes zero, where h is the pressure head.
- **Initial Water Content (THTI) [$L^3 L^{-3}$]:** The water content at the beginning of the simulation. THTI is needed only if the first stress period is transient or if the SPECIFYTHTI box in the Options tab (see below) is checked.

o **Cell Properties** (for Cell-by-Cell input method), **Polygon Properties** (for Polygon input method), or **Vertex Properties** (for Polyline input method)

- **Infiltration Rate (FINF) [LT^{-1}]:** This is the specified infiltration rate.
- **Potential ET (PET) [LT^{-1}]:** Potential evapotranspiration flux.
- **ET Extinction Depth (EXTDP) [L]:** The quantity of ET removed from a cell is limited by the volume of water stored in the unsaturated zone above the extinction depth. If groundwater is within the ET extinction depth, then the rate removed is based on a linear decrease in the maximum rate at land surface and zero at the ET extinction depth.
- **ET Extinction Water Content (EXTWC) [$L^3 L^{-3}$]:** The water content below which ET cannot be removed from the unsaturated zone.
- **Parameter Number** is used to group cells, where the FINF value is to be estimated by PEST. See *To define an estimable parameter* in Section 3.8.4 for details.

- **Options Tab**

o **IUZFOPT:** Check this box to route water through unsaturated zone (i.e., IUZFOPT = 1 if checked; otherwise IUZFOPT = 0).

o **IRUNFLG:** Check this box to route ground water that discharges to land surface to stream segments or lakes as specified in the IRUNBND array.

o **IETFLG:** Specifies whether evapotranspiration (ET) will be simulated. ET will be simulated if this box is checked, otherwise it will not be simulated.

o **NTRAIL2 [-]:** This is the number of trailing waves used to define the water-content profile following a decrease in the infiltration rate.

o **NSETS2 [-]:** This is the number of wave sets used to simulate multiple infiltration periods.

o **SURFDEP [L]:** This is the average surface depression depth of the UZF cells.

o **NOSURFLEAK:** When the head is higher than the land surface, water seepage to the land surface may be removed from the groundwater system if this box is cleared.

- o **SPECIFYTHTR**: If this box is checked, the residual water content (THTR) for each vertical column of cells is specified. Otherwise, the residual water content will be calculated.
- o **SPECIFYTHTI:** If this box is checked, the initial water content (THTI) for each vertical column of cells is always specified, regardless of whether the first stress period is transient or steady-state.

3.8.1.1.20. Well (WEL)

The Well (WEL) Package is designed to simulate features such as wells that withdraw water from or add water to the aquifer at a constant rate during a stress period, where the rate is independent of both the cell area and the head in the cell. The Package can be used to simulate any features for which the recharge or discharge can be directly specified. Consider using the MNW1 Package (Section 3.8.1.1.10) for wells that penetrate multiple model layers.

The required input parameters are listed below. For large pumping data sets, consider using the **Tools > Package > Append Well** function described in Sections 3.5.20 and 5.1.16.

1. **All input methods** include a Simulation Settings group that contains the following option:

   - **Include Concentration Data in the SSM Package of MT3D/SEAWAT:** If this box is checked, the values entered to **Concentration (MT3D/SEAWAT) [ML^{-3}]** are used as source water concentration. If this box is not checked, the concentration of the source water is assumed to be zero.

2. **Cell-by-cell input method:** Figure 81 shows the dialog box for specifying cell properties.

   - **Flow Rate (Q) [L^{3}T^{-1}]:** Negative values are used to indicate pumping wells, while positive cell values indicate injection wells. The injection or pumping rate of a well is independent of both the cell area and the hydraulic head in the cell. MODFLOW assumes that a well penetrates the full thickness of the cell. To simulate wells that penetrate more than one model layer with the WEL Package, a flow rate must be specified for each penetrated layer. The total flow rate for a multi-layer well is equal to the sum of flow rates of individual layers.
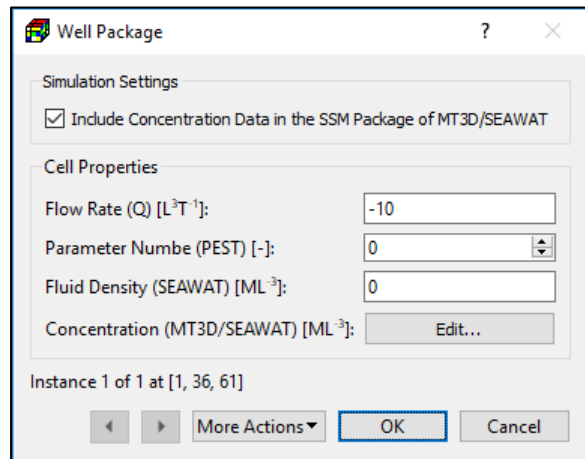
Figure 81. The Well Package dialog box for specifying cell properties

For confined layers, the flow rate for each layer Q_k can be approximately calculated by dividing the total rate (Q_{total}) in proportion to the layer transmissivities (McDonald, et al., 1988):

$$Q_k = Q_{total} \cdot \frac{T_k}{\Sigma T}$$
<div align="right">(34)</div>

where

T_k is the transmissivity of layer k, and

ΣT is the sum of the transmissivity values of all layers penetrated by the multi-layer well.

- Another possibility to simulate a multi-layer well with the WEL Package is to set a large vertical hydraulic conductivity (or vertical leakance), e.g. 1 m/s, to all cells of the well. The total pumping rate is then assigned to the lowest cell of the well. For display purposes, a very small pumping rate (e.g., $-1 \times 10^{-10} \, m^3/s$) can be assigned to other cells of the well. In this way, the exact extraction rate from each penetrated layer can be obtained by using ZoneBudget. See Section 3.8.2 for details about ZoneBudget.

- **Parameter Number** is used to group cells, where the Q value is to be estimated by PEST. See *To define an estimable parameter* in Section 3.8.4 for details.

- **Fluid Density (SEAWAT) [ML⁻³]** is the density of injected fluid and is used by SEAWAT only if it is running in the uncoupled mode (i.e., the density-effect of all species are turned off, see Section 3.8.3.1) and WELDENS (see Figure 99. The VDF tab of the Transport Settings dialog box) is set as *User-Specified in the WEL Package*.

- **Concentration (MT3D/SEAWAT) [ML⁻³]:** Click the Edit button to open a Concentration dialog box (Figure 42) that allows you to specify the injected water concentration of up to 100 species. You can either enter individual concentration values to the table directly or click the *Set Value* button to enter a uniform value for all species. The entered concentration values may be used by the SSM Package of MT3D or SEAWAT.

3. **Polyline input method:** Figure 82 shows the dialog box for specify the following data to one or more vertices of a polyline. These vertex data can then be interpolated to model cells following the rules described in Section 3.3.2.2 and additional rules below.

   - **Flow Rate per Unit Length [L²T⁻¹]** is interpolated to the cells along the polyline. For each of those cells, the interpolated cell value Q_l is multiplied with the length of the polyline within the cell to obtain the flow rate Q:

$$Q = Q_l \cdot L_c$$
<div align="right">(35)</div>

where
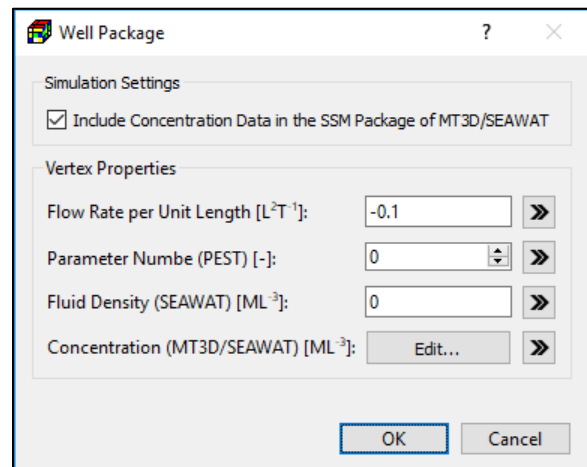
Figure 82. The Well Package dialog box for specifying vertex properties

Q_l is the flow rate per unit length at a given cell, and

L_c is the length of the polyline within the cell.

- **The other parameter values** are interpolated to cells along the polyline and the interpolated values are used as the input data to those cells.

4. **Polygon input method:** Figure 83 shows the dialog box for specify the following data are to a polygon. These data can then be assigned to model cells following the rules described in Section 3.3.2.3 and additional rules below.

- **Flow Rate per Unit Area [T⁻¹]** is assigned to the cells within the polygon. For each of those cells, the cell value Q_a is multiplied with the cell area to obtain the flow rate Q:

$$Q = Q_a \cdot Area_c \qquad (36)$$

where

Figure 83. The Well Package dialog box for specifying polygon properties

Q_a is the flow rate per unit area at a given cell, and

$Area_c$ is the area of the cell.

- **The other parameter values** are used as the input data to the cells within the polygon.

3.8.1.1.21. Wetting Threshold

When a model cell of an unconfined or convertible layer falls dry (i.e., its head falls below the cell bottom), the cell is set as a no-flow cell (with IBOUND = 0) and all conductance values to the cell are set to zero. As the simulation proceeds, a dry cell remains inactive even if the head at neighboring cells rise above its bottom.

The BCF or LPF Package uses the Wetting Threshold (THRESH) to overcome this problem. At the start of a solution iteration, a dry cell may be converted to wet if h ≥ BOT + |THRESH|, where h is the head value at an adjacent cell, BOT is the bottom elevation of the dry cell. When a dry cell is wetted, its IBOUND value is set to 1 (which indicates a variable-head cell), its original conductance values are restored, and its head value is set to a value slightly above the cell bottom.

The required input parameters for all input methods are identical and given below.

1. **All input method:** Figure 84 shows the dialog box for specifying cell, vertex, or polygon properties.

- Interval (IWETIT) is the iteration interval for attempting to wet cells. Wetting is attempted every IWETIT iteration. If the PCG solver is used, this applies to outer iterations, not inner iterations.

  The reason for adjusting IWETIT is that the wetting of cells sometimes produces erroneous head changes in neighboring cells during the succeeding iteration, which

Figure 84. The Wetting Capability dialog box

  may cause erroneous conversions of those cells. Waiting a few iterations until heads have had a chance to adjust before testing for additional conversions can prevent these errors. When setting IWETIT greater than one, there is some risk that cells may be prevented from correctly converting from dry to wet. If the solution for a time step is obtained in less than IWETIT iterations, then there will be no check during that time step to see if cells should be converted from dry to wet. The potential for this problem to occur is greater in transient simulations, which frequently require only a few iterations for a time step.

- **Factor (WETFCT)** is used in the calculation of the initial head at a cell that is converted from dry to wet.

- **Initial Head at Rewetted Cells:** This determines which equation is used to define the initial head (h) at the cell that becomes wet.

$$h = BOT + WETFCT \cdot (h_n - BOT) \tag{37}$$

$$h = BOT + WETFCT \cdot |THRESH| \tag{38}$$

$where$

   BOT is the bottom elevation of the cell,

   h_n is the head at an adjacent cell, and

   $|THRESH|$ is the absolute value of the wetting threshold at the cell.

The initial estimate of head at a cell that converts to wet is theoretically unimportant because the solver should calculate the correct value in subsequent iterations. In practice, however, the initial estimate is often important for solver efficiency; that is, if a poor choice is made, the solver convergence may be slower than optimum. A bad choice for initial head also can cause the cell to oscillate between wet and dry.

- **Wetting Threshold (THRESH):** When the head at an adjacent cell equals or exceeds BOT + |THRESH| of a dry cell, the dry cell is wetted. The sign of THRESH is used as a flag:

  o If THRESH < 0, only the cell below a dry cell can cause the cell to become wet.

  o If THRESH > 0, the cell below a dry cell and the four horizontally adjacent cells can cause a cell to become wet.

  o If THRESH is 0, the cell cannot be wetted.

  A primary difficulty with the rewetting approach is that the value of THRESH must be determined by trial and error. If |THRESH| is too low, a cell may be incorrectly converted to wet. That is, a cell may convert to wet and then reconvert to dry in later solver iterations because the head does not stay above the bottom elevation. This cycle of converting between wet and dry conditions can repeat indefinitely, preventing the solver from converging. Larger values of |THRESH| can avoid repeated conversion between wet and dry, but they increase the non-uniqueness of the solution (McDonald, et al., 1991).

The method of wetting and drying cells used in the BCF and LPF Packages can cause convergence problems with the iterative solvers. Symptoms of a convergence problem are slow convergence or divergence combined with the frequent wetting and drying of the same cells. For example, a well-cell with large pumping rate could cause the cell (and perhaps also neighboring cells) to fall dry. Thus, the pumping at that cell is switched off, the water table rises due to lack of pumping, the dry cell is wetted, and the pumping is re-established. The cycle repeats. Similar problems may occur near sinks or at places with small saturated thickness. You can detect such situations by examining the model run listing file with *Models > MODFLOW > View > Run Listing File*. A message is printed to that file each time a cell converts. Some options to mitigate the convergence problems are

1. Modify the settings
   - Set THRESH < 0, so that wetting can only be from below.
   - Increase IWETIT.
   - Use another equation for calculating the initial head at rewetted cells.
   - Increase the absolute value of THRESH.
2. Use a different solver or change solver settings.
3. Modify the vertical discretization such that only few cells will fall dry.
4. Decrease flow rates of sinks, such as pumping rates of wells.

3.8.1.2. Solvers

To calculate hydraulic heads, MODFLOW prepares one finite difference equation for each cell, expressing the relationship between the head at a node and the heads at each of the six adjacent nodes at the end of each time step. Because each equation may involve up to seven unknown

values of head, and because the set of unknown head values changes from one equation to the next through the grid, the equations for the entire grid must be solved simultaneously at each time step. The system of simultaneous finite difference linear equations can be expressed in matrix notation as

$$\underline{A} \cdot \underline{x} = \underline{b} \tag{39}$$

where $\underline{A}$ is a coefficient matrix assembled by MODFLOW using user-specified model data; $\underline{b}$ is a vector of defined flows, terms associated with head-dependent boundary conditions and storage terms at individual cells; $\underline{x}$ is a vector of hydraulic heads at individual cells. During a MODFLOW run, the vector $\underline{x}$ is solved with one of the supported solvers.

3.8.1.2.1. Direct (DE4)

The Direct Solution (DE4) Package (Harbaugh, 1995) uses Gaussian elimination with an alternating diagonal equation numbering scheme that is more efficient than the standard method of equation numbering. A direct solver is the most efficient when solving small, linear problems. Although direct solvers require more memory and typically require more computational effort than iterative solvers, the direct solver may execute faster than an iterative solver in some situations.

This package is deactivated if the Upstream Weighting (UPW) Package is selected as the internal flow package, see Section 3.4.6 for details.

Figure 85 shows the dialog box for specifying the following required input parameters:

1. **Problem Type (IFREQ):** The choice of problem type affects the efficiency of solution; significant work can be avoided if it is known that the coefficient matrix $\underline{A}$ (Equation 39) remains constant all or part of the time.
   - **Linear** indicates that the flow equations are linear, but coefficients of simulated head for some stress terms may change at the start of each stress period. Examples of coefficients of simulated head for stress terms are riverbed conductance, drain conductance, maximum evapotranspiration rate, evapotranspiration extinction depth, and general-head boundary conductance.

- **Nonlinear** indicates that a non-linear flow equation is being solved, which means that some terms in _A_ depend on simulated head. Example of head dependent terms are transmissivity for water-table layers, which is based on the saturated thickness; flow terms for rivers, drains, and evapotranspiration convert between head dependent flow and constant flow; and the change in storage coefficient when a cell converts between
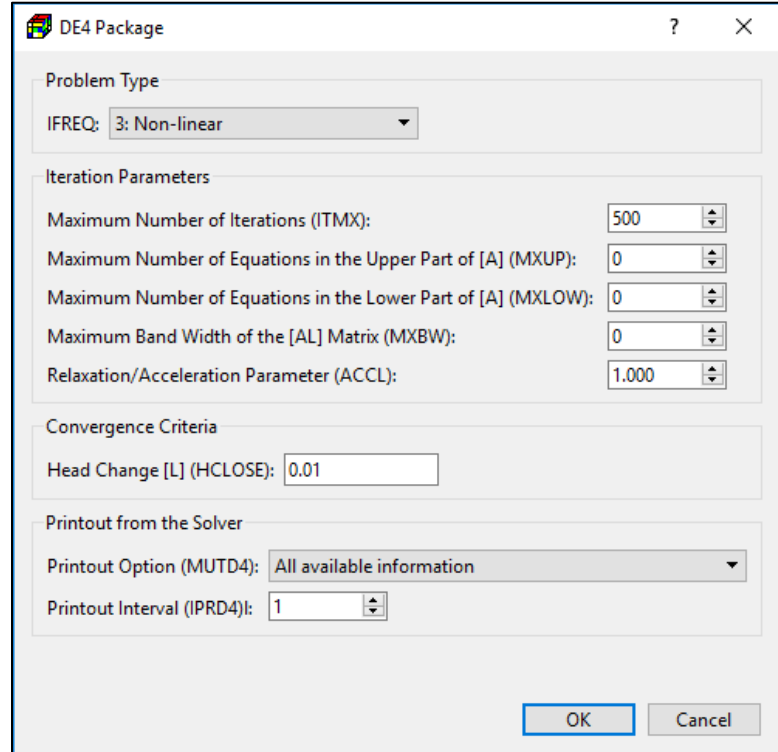
Figure 85. The DE4 Package dialog box

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

2. **Iteration Parameters**

- **Maximum Number of Iterations (ITMX)** is the maximum number of iterations in each time step. Specify ITMX = 1 if iteration is not desired. Ideally iteration would not be required for direct solution; however, it is necessary to iterate if the flow equation is nonlinear or if computer precision limitations result in inaccurate calculations as indicated by a large water budget error.

- **Maximum Number of Equations in the Upper Part of [A] (MXUP)** is the maximum number of equations in the upper part of the equations to be solved. This value impacts the amount of memory used by the solver. If specified as 0, the solver will calculate MXUP as half the number of cells in the model, which is an upper limit.

- **Maximum Number of Equations in the Lower Part of [A] (MXLOW)** is the maximum number of equations in the lower part of the equations to be solved. This value impacts the amount of memory used by the solver. If specified as 0, the solver will calculate MXLOW as half the number of cells in the model, which is an upper limit.

- **Maximum Band Width of the [AL] Matrix (MXBW)** is the maximum band width plus 1 of the [AL] matrix. This value impacts the amount of memory used by the solver. If specified as 0, the solver will calculate MXBW as the product of the two smallest grid dimensions plus 1, which is an upper limit.

- **Relaxation/Acceleration Parameter (ACCL)** is a multiplier for the computed head change for each iteration. Normally this value is 1. A value greater than 1 may be useful for improving the rate of convergence when using external iteration to solve non-linear problems. ACCL should always be 1 for linear problems. When ITMX=1, the solver changes ACCL to 1 regardless of the input value.

3. **Convergence Criteria**
   - **Head Change [L] (HCLOSE):** This is the head change criterion for convergence. When the maximum absolute value of head change from all nodes during an iteration is less than or equal to HCLOSE, iteration stops.

4. **Printout from the Solver**
   - **Printout Option (MUTD4):** This controls printing of convergence information from the solver.
     - **All available information**: The maximum head change and residual (positive or negative) are saved in the run listing file for each iteration of a time step whenever the time step is an even multiple of Printout Interval.
     - **The number of iterations only:** The printout of maximum head change and residual is suppressed.
     - **None**: Suppress all printout from the solver.
   - **Printout Interval (IPRD4):** This is the time step interval for printing out convergence information when iterating (ITMX > 1).

3.8.1.2.2. Strongly Implicit Procedure (SIP)

This package is deactivated if the Upstream Weighting (UPW) Package is selected as the internal flow package, see Section 3.4.6 for details.

Figure 86 shows the dialog box for specifying the following required input parameters:

1. **Iteration Parameters**

- **Maximum Number of Iterations (MXITER)** is the maximum number of times through the iteration loop within a time step to solve the system of equations.

- **Number of Iteration Parameters (NPARM)** is the number of iteration variables to be used. Five variables are generally sufficient.

- **Acceleration Parameter (ACCL)** is the acceleration variable. It must be greater than zero and is generally equal to one. If a zero is entered, it is changed to one by the solver.
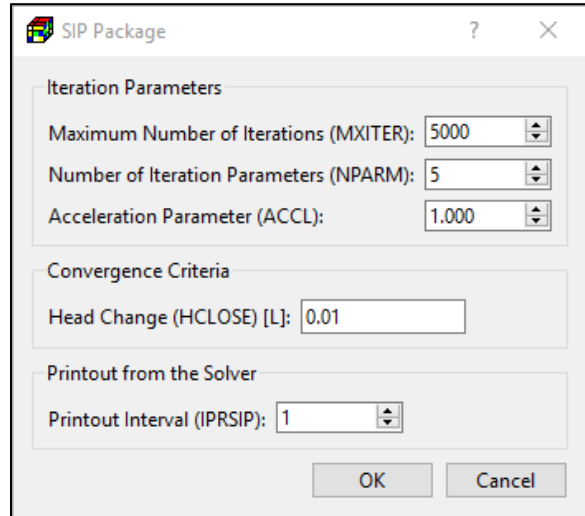
Figure 86. The SIP Package dialog box

2. **Convergence Criteria**

- **Head Change (HCLOSE) [L]:** This is the head change criterion for convergence. When the maximum absolute value of head change from all nodes during an iteration is less than or equal to HCLOSE, iteration stops.

3. **Printout from the Solver**

- **Printout Interval (IPRSIP):** The maximum head change (positive or negative) is printed for each iteration of a time step whenever the time step is an even multiple of IPRSIP.

3.8.1.2.3. Geometric Multigrid (GMG)

This package is deactivated if the Upstream Weighting (UPW) Package is selected as the internal flow package, see Section 3.4.6 for details.

Figure 87 shows the dialog box for specifying the following required input parameters of the Geometric Multigrid Solver (GMG) Package (Wilson, et al., 2004).

1. **Preconditioning Method**

- **Smoother Type (ISM):** ISM controls the type of smoother used in the multigrid preconditioner.

  o **ILU Smoothing:** Select this option to implement ILU(0) smoothing in the multigrid preconditioner. This smoothing requires an additional vector on each multigrid level to store the pivots in the ILU factorization.

o **Symmetric Gauss-Seidel (SGS) Smoothing:** Select this option to implement the Symmetric Gauss-Seidel (SGS) smoothing in the multigrid preconditioner. No additional storage is required for this smoother; users may want to use this option if available memory is exceeded or nearly exceeded when using ILU Smoothing. Using SGS smoothing is not as robust as ILU
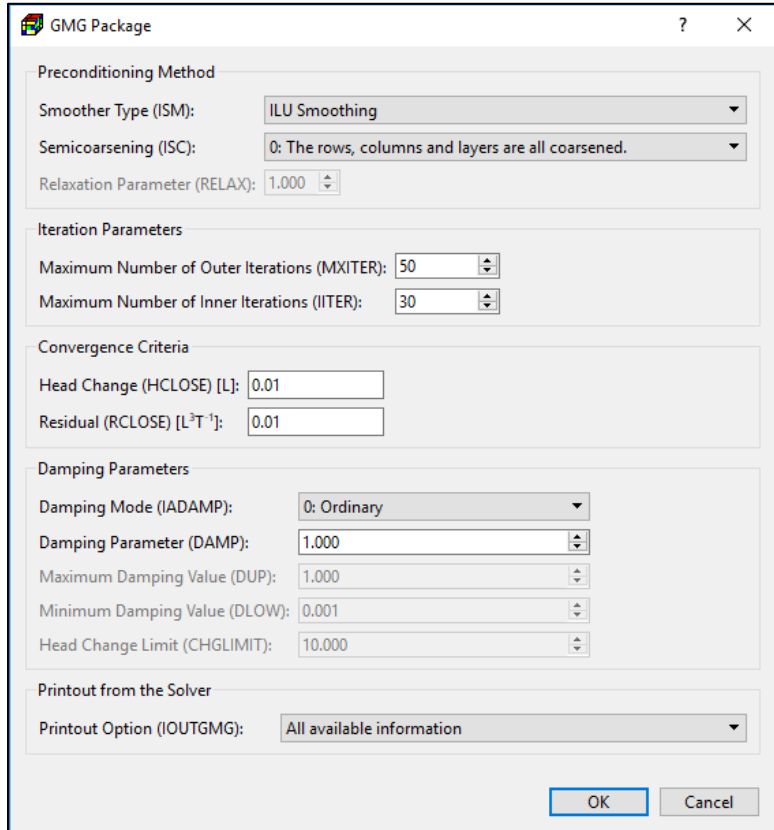
Figure 87. The GMG Package dialog box

smoothing; additional iterations are likely to be required in reducing the residuals. In extreme cases, the solver may fail to converge as the residuals cannot be reduced sufficiently.

- **Semicoarsening (ISC):** This option controls semi-coarsening in the multigrid preconditioner. The available options and their meanings are given as follows:

o The rows, columns and layers are all coarsened.
o The rows and columns are coarsened, but the layers are not.
o The columns and layers are coarsened, but the rows are not.
o The rows and layers are coarsened, but the columns are not.
o No coarsening takes place.

Typically, the first or second option should be selected. In the case that there are large vertical variations in the hydraulic conductivities, then the second option should be used. If no coarsening is implemented, the GMG solver is comparable to the PCG ILU(0) solver and uses the least amount of memory.

- **Relaxation Parameter (RELAX)** is a relaxation parameter for the ILU preconditioned conjugate gradient method. The RELAX parameter can be used to improve the spectral condition number of the ILU preconditioned system. The value of RELAX

should be approximately one. However, the relaxation parameter can cause the factorization to break down. If this happens, then the GMG solver will report an assembly error and a value smaller than one for RELAX should be tried.

2. **Iteration Parameters**

- **Maximum Number of Outer Iterations (MXITER):** For linear problems, MXITER can be set to 1. For nonlinear problems, MXITER needs to be larger, but rarely more than 100.

- **Maximum Number of Inner Iterations (IITER)** is the maximum number of PCG iterations for each linear solution. A value of 100 is typically sufficient. It is frequently useful to specify a smaller number for nonlinear problems to prevent an excessive number of inner iterations.

3. **Convergence Criteria**

- **Head Change (HCLOSE) [L]** is the head change convergence criterion for nonlinear problems. After each linear solve (inner iteration), the maximum of the head change is compared against HCLOSE. HCLOSE can be set to a large number for linear problems; HCLOSE is ignored if MXITER=1.

- **Residual (RCLOSE) [L^{3}T^{-1}]** is the residual convergence criterion for the inner iteration. Typically, RCLOSE is set to the same value as HCLOSE. If RCLOSE is set too high, then additional outer iterations may be required due to the linear equation not being solved with sufficient accuracy. On the other hand, a too restrictive setting for RCLOSE for nonlinear problems may force an unnecessarily accurate linear solution.

4. **Damping Parameters**

- **Damping Mode (IADAMP)** is a flag that controls adaptive damping. The possible values of IADAMP and their meanings are as follows:

  o **0: Ordinary:** the value assigned to DAMP is used as a constant damping parameter.
  o **1: Cooley's method:** the value of DAMP is used for the first nonlinear iteration. The damping parameter is adaptively varied based on the head change, using Cooley's method as described in (Mehl, et al., 2001), for subsequent iterations.
  o **2. Relative reduced residual method:** the relative reduced residual damping method documented in (Mehl, et al., 2001) and modified by (Banta, 2006) is used.

  When IADAMP is specified as 2 and the value specified for DAMP is less than 0.5, the closure criterion for the inner iterations (DRCLOSE) is assigned simply as RCLOSE. When DAMP is between 0.5 and 1.0, inclusive, or when IADAMP is specified as 0 or 1, DRCLOSE is calculated according to equation 20 on p. 9 of (Wilson, et al., 2004)

- **Damping Parameter (DAMP)** is the value of the damping parameter. For linear problems, a value of 1.0 should be used. For nonlinear problems, a value less than 1.0 but greater than 0.0 may be necessary to achieve convergence. A typical value for nonlinear problems is 0.5. Damping also helps control the convergence criterion of the linear solve to alleviate excessive PCG iterations.

- **Maximum Damping Value (DUP)** is the maximum damping value that should be applied at any iteration when the solver is not oscillating; it is dimensionless. An appropriate value for DUP will be problem-dependent. For moderately nonlinear problems, reasonable values for DUP would be in the range 0.5 to 1.0. For a highly nonlinear problem, a reasonable value for DUP could be as small as 0.1. When the solver is oscillating, a damping value as large as 2.0 × DUP may be applied.

- **Minimum Damping Value (DLOW)** is the minimum damping value to be generated by the adaptive-damping procedure; it is dimensionless. An appropriate value for DLOW will be problem-dependent and will be smaller than the value specified for DUP. For a highly nonlinear problem, an appropriate value for DLOW might be as small as 0.001.

- **Head Change Limit (CHGLIMIT)** is the maximum allowed head change at any cell between outer iterations.

5. **Printout from the Solver**

    - **Printout Option (IOUTGMG):** This controls printing of convergence information from the solver. Available options are

        o Only the solver inputs
        o All available information
        o The convergence history of the PCG iteration

3.8.1.2.4. Preconditioned Conjugate Gradient (PCG)

The Preconditioned Conjugate-Gradient Solver (PCG) Package is fully documented in (Hill, 1990). The PCG solver incorporates two forms of the Preconditioned Conjugate-Gradient method: the Modified Incomplete Cholesky and the Polynomial methods. Knowledge of the details of these methods generally is not necessary. The most important aspect is that the Modified Incomplete Cholesky method is almost always faster. The Polynomial method is potentially faster only on parallel computers where some of the work can be performed simultaneously on multiple processors.

This package is deactivated if the Upstream Weighting (UPW) Package is selected as the internal flow package, see Section 3.4.6 for details.

Figure 88 shows the dialog box for specifying the following required input parameters:

1. **Preconditioning Method**

    - **NPCOND:** This is the matrix preconditioning method. The available options are

        o Modified Incomplete Cholesky (for use on scalar computers)
        o Neuman series polynomial (for use on parallel computers)

    - **NBPOL**: This is used with the Neuman series polynomial preconditioning method. Checking this box to calculate the estimate of the upper bound on the maximum

eigenvalue. If this box is cleared, the estimate is set as 2. Convergence is generally insensitive to this parameter.

2. **Iteration Parameters**

   • **Maximum Number of Outer Iterations (MXITER):** For a linear problem MXITER should be 1, unless more than 50 inner iterations are required, when MXITER could be as large as 10. A larger number (generally less than 100) is required for a nonlinear problem.
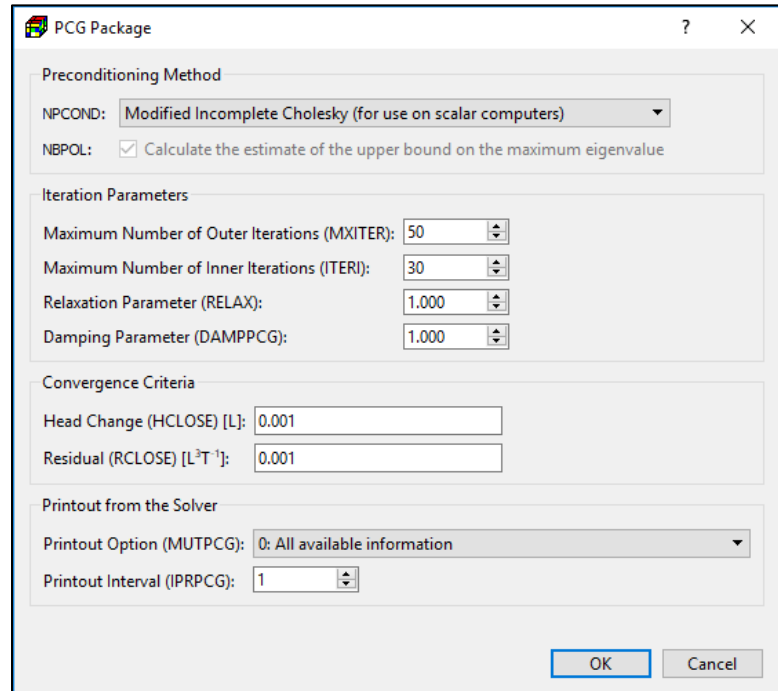
Figure 88. The PCG Package dialog box

For a linear problem, a single outer iteration with many inner iterations theoretically is adequate, but a few outer iterations should be used for large (greater than 10,000 cells) linear models. For numerical reasons described in p. 8 of (Hill, 1990), the outer iterations improve the accuracy of large linear problems.

• **Maximum Number of Inner Iterations (ITERI):** For nonlinear problems, ITERI usually ranges from 10 to 30; a value of 30 will be sufficient for most linear problems.

Nonlinear problems generally run most efficiently with five or more outer iterations and a large number of inner iterations (20 or more). The solution process becomes inefficient if the nonlinear terms are reformulated frequently by having a small (less than 20) value for ITER1.

• **Relaxation Parameter (RELAX):** This is the relaxation parameter used with the Modified Incomplete Cholesky preconditioning method. Usually, RELAX=1.0, but for some problems a value of 0.99, 0.98, or 0.97 will reduce the number of iterations required for convergence.

• **Damping Parameter (DAMPPCG):** Values less than 1.0 can be used to aid convergence in nonlinear problems.

3. **Convergence Criteria**

   • **Head Change (HCLOSE) [L]** is the head change criterion for convergence. When the maximum absolute value of head change from all nodes during an iteration is less than or equal to HCLOSE, and the criterion for RCLOSE is also satisfied (see below), iteration stops.

- **Residual (RCLOSE) [L³T⁻¹]** is the residual criterion for convergence. When the maximum absolute value of the residual at all nodes during an iteration is less than or equal to RCLOSE, and the criterion for HCLOSE is also satisfied (see above), iteration stops. For nonlinear problems, convergence is achieved when the convergence criteria are satisfied for the first inner iteration.

4. **Printout from the Solver**

   - **Printout Option (MUTPCG)** is a flag that controls printing of convergence information from the solver:

     o **0: All available information:** Print tables of maximum head change and residual each iteration.
     o **1: The number of iterations only:** Print only the total number of iterations
     o **2: None**: No Printing.
     o 3: Print as for 0, but only if solver convergence fails

   - **Printout Interval (IPRPCG):** The extreme head change and residual (positive or negative) 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 value of the printout interval.

3.8.1.2.5. PCG with Improved Nonlinear Control (PCGN)

The principal objective of the preconditioned conjugate gradient with improved nonlinear control (PCGN) Package (Naff, et al., 2008) is to provide the modeler with more options when faced with a poorly converging nonlinear problem. Picard iteration is used to solve nonlinear ground-water flow equations by iteratively solving a linear approximation of the nonlinear equations. The linear solution is provided by means of the preconditioned conjugate gradient algorithm where preconditioning is provided by the modified incomplete Cholesky algorithm. The incomplete Cholesky scheme incorporates two levels of fill, 0 and 1, in which the pivots can be modified so that the row sums of the preconditioning matrix and the original matrix are approximately equal. A relaxation factor is used to implement the modified pivots, which determines the degree of modification allowed. The preconditioned conjugate gradient method is coupled with Picard iteration to efficiently solve the nonlinear equations associated with many ground-water flow problems.

This package is deactivated if the Upstream Weighting (UPW) Package is selected as the internal flow package, see Section 3.4.6 for details.

Figure 89 shows the dialog box for specifying the following required input parameters:

1. **Iteration Parameters**
   - **Maximum Number of Outer Iterations (ITER_MO):** For nonlinear problems, this variable must be set to some number greater than one, depending on the problem

size and degree of nonlinearity. If this variable is set to 1, then the PCGN solver assumes that the problem is linear.

- **Maximum Number of Inner Iterations (ITER_MI):** Generally, this variable is set to some number greater than one, depending on the matrix size, degree of convergence called for, and the nature of the problem. For a nonlinear problem, this variable should be set large enough

- **Relaxation Parameter (RELAX)** is used with the modified incomplete Cholesky preconditioning method. A value of RELAX between 0.9 and 1 is generally advised for most problems.
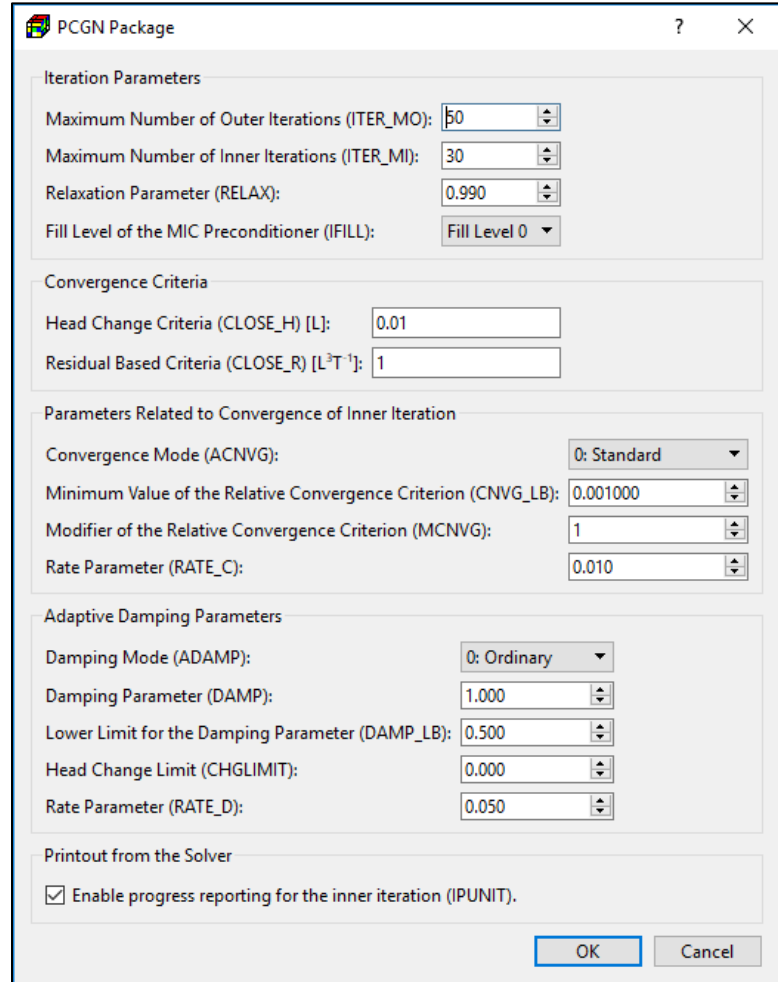
Figure 89. The PCGN Package dialog box

- **Fill Level of the MIC Preconditioner (IFILL):** Generally, the higher the fill level, the more preconditioning imparted by a modified incomplete Cholesky preconditioner. For problems where the matrix equation is not well behaved or for a nonlinear problem where convergence is not easily achieved, a fill level of 1 may provide the additional preconditioning necessary to obtain convergence.

2. **Convergence Criteria**

- **Residual Based Criteria (CLOSE_R) [L³T⁻¹]:** This parameter is used differently, depending on whether it is applied to a linear or nonlinear problem:

  o **ITER_MO = 1**: CLOSE_R is used as the value in the absolute convergence criterion for quitting the PCG iterative solver. CLOSE_R is compared to the square root of the weighted residual norm v. This norm is defined as $v = r^T M^{-1} r$, where M represents the preconditioning matrix with the PCG algorithm and r is a vector of

residuals. If $\sqrt{v}$ is less than CLOSE_R, then the linear PCG iterative solve is said to have converged.

- o **ITER_MO > 1**: For a nonlinear problem, CLOSE_R is used as a criterion for quitting the Picard (outer) iteration. CLOSE_R is compared to the square root of the inner product of the residuals (the residual norm), $[r^T r]^{1/2}$, as calculated on entry to the PCG solver at the beginning of every Picard iteration. If this norm is less than CLOSE_R, then the Picard iteration is considered to have converged.

- **Head Change Criteria (CLOSE_H) [L]:** CLOSE_H is used as an alternate stopping criterion for the Picard iteration needed to solve a nonlinear problem. The maximum value of the head change is obtained for each Picard iteration, after completion of the inner, PCG iteration. If this maximum head change is less than CLOSE_H, then the Picard iteration is considered tentatively to have converged. However, as nonlinear problems can demonstrate oscillation in the head solution, the Picard iteration is not declared to have converged unless the maximum head change is less than CLOSE_H for three Picard iterations. If these Picard iterations are sequential, then a good solution is assumed to have been obtained. If the Picard iterations are not sequential, then a warning is issued advising that the convergence is conditional and the user is urged to examine the mass balance of the solution.

3. **Parameters Related to Convergence of Inner Iteration**

- **Convergence Mode (ACNVG):** ACNVG defines the mode of convergence applied to the PCG solver. In general, the relative stopping criterion for PCG iteration is $v_i < \varepsilon v_0$ where v_0 is the weighted residual norm on entry to the PCG solver, ε is the relative convergence parameter, and v_i is the same norm at PCG iteration i. The available convergence modes are:

  - o **ACNVG=0**: The standard convergence scheme is employed. The standard relative convergence is denoted by ε_s and usually takes the value 0.1; this value is assigned to the relative convergence ε. No additional variables are used.
  - o **ACNVG=1:** Adaptive convergence is employed. The adaptive convergence scheme adjusts the relative convergence ε of the PCG iteration based on a measure of the nonlinearity of the problem. Under this scheme, ε is allowed to vary such that CNVG_LB $< \varepsilon < \varepsilon_s$ where the exact value of ε is dependent on the measure of nonlinearity. This option requires a valid value for variable CNVG_LB.
  - o **ACNVG=2:** Enhanced convergence is employed. If the variable enhancement option is employed (RATE_C > 0), then ε_s is taken as the upper limit for ε. This option requires valid values for variables MCNVG and RATE_C.

- **Minimum Value of the Relative Convergence Criterion (CNVG_LB)** is used only in convergence mode ACNVG = 1. CNVG_LB is the minimum value that the relative convergence ε can take under the self-adjusting convergence option. The objective here is to prevent ε from becoming so small that the PCG solver takes an excessive

number of iterations. Valid range for variable: 0 < CNVG_LB < ε_s; a value of CNVG_LB = 0.001 usually produces reasonable results.

- **Modifier of the Relative Convergence Criterion (MCNVG)** is used only in convergence mode ACNVG = 2. MCNVG increases the relative PCG convergence criteria by a power equal to MCNVG; that is, letting p = MCNVG, then the relative convergence criterion ε is enhanced such that $\varepsilon = \varepsilon_s^p$ where $0 < p \leq 6$. If MCNVG is set to a value greater than 6, then PCGN resets MCNVG = 6 and issues a warning message. If RATE_C = 0, then this enhanced relative convergence criterion is applied uniformly throughout the simulation; the relative convergence, in this case, is not adjusted for stress changes in the simulation. MCNVG must be set to a value greater than zero when ACNVG = 2; otherwise a data error is declared and ACNVG is reset to zero.

- **Rate Parameter (RATE_C)** is used only in convergence mode ACNVG = 2; this option results in variable enhancement of ε. If 0 < RATE_C < 1, then enhanced relative convergence is allowed to decrease by increasing ε as follows: $\varepsilon_j = \varepsilon_{j-1} + RATE\_C \cdot \varepsilon_{j-1}$ where j is the Picard iteration number; this change in ε occurs so long as the Picard iteration progresses satisfactorily. If RATE_C $\leq$ 0, then the value of ε set by MCNVG remains unchanged through the Picard iteration. It should be emphasized that RATE_C must have a value greater than 0 for the variable enhancement to be effective; otherwise ε remains constant. The assumption here is that a better solution of the linear equations is needed initially to improve the nonlinear Picard solution, but that this need abates with additional Picard iterations. Typical values for RATE_C are 0.01 < RATE_C < 0.1, although larger or smaller values may be used.

4. **Adaptive Damping Parameters**
   - **Damping Mode (ADAMP)** defines the mode of damping applied to the linear solution. In general, damping determines how much of the head changes vector Δj shall be applied to the hydraulic head vector hj in Picard iteration j: $h_j = h_{j-1} + \theta \Delta_j$, where θ is the damping parameter. The available damping modes are:

     o ADAMP = 0: Ordinary damping is employed and a constant value of damping parameter θ = DAMP will be used throughout the Picard iteration. This option requires a valid value for DAMP.

     o ADAMP = 1: Adaptive damping is employed; Adaptive damping changes the damping parameter θ in response to the difficulty the nonlinear solver encounters in solving a given problem. Essentially, the nonlinear solver looks to increase θ should the convergence of the Picard iteration proceed satisfactorily, but otherwise causes θ to decrease. Adaptive damping can be useful for problems that do not converge readily, but otherwise should be avoided as it generally requires more total iterations. This option requires valid values for variables DAMP, DAMP_LB, RATE_D, and CHGLIMIT. Adaptive damping also admits the possibility of directly limiting the maximum head change applicable to update the hydraulic

heads; see CHGLIMIT below. If this option is not desired, then CHGLIMIT should be set to zero.

- o **ADAMP = 2:** Enhanced damping algorithm in which the value of θ is increased (but never decreased) provided the Picard iteration is proceeding satisfactorily. This enhanced damping allows θ to increase from a minimum value to a maximum value DAMP by a rate equal to RATE_D. The minimum value in the first stress period is DAMP_LB; for subsequent stress periods, it is the geometric mean of DAMP and DAMP_LB. This option requires valid values for DAMP, DAMP_LB, and RATE_D.

- **Damping Parameter (DAMP)** restricts the damping parameter θ; generally, 0 < DAMP < 1. Its function for the various modes of ADAMP are:

  - o **ADAMP = 0:** The damping parameter θ takes on the value DAMP and is maintained constant throughout the simulation.
  - o **ADAMP > 0:** The value of DAMP will be treated as the upper limit for θ in the enhanced damping or adaptive damping algorithms.

- **Lower Limit for the Damping Parameter (DAMP_LB)** represents a bound placed on θ; generally, 0 < DAMP_LB < DAMP. For the various modes of ADAMP > 0, DAMP_LB serves the following purposes:

  - o **ADAMP = 1:** In the adaptive damping algorithm, DAMP_LB represents the lower limit to which θ, under adverse adaptive damping conditions, will be allowed to fall.
  - o **ADAMP = 2:** In the enhanced damping algorithm, DAMP_LB is the starting value (or a component of the starting value) for the damping parameter θ used in the initial Picard iteration of every stress period.

- **Head Change Limit (CHGLIMIT)** limits the maximum head change applicable to the updated hydraulic heads in a Picard iteration. Provided that the current damping factor is greater than the ratio of CHGLIMIT to the maximum head change and that this ratio is less than one, then the damping factor is reset to the value of the ratio. This option is available only in association with adaptive damping: ACNVG = 1. If CHGLIMIT = 0.0, then adaptive damping proceeds without this feature.

- **Rate Parameter (RATE_D):** Generally, 0 < RATE_D < 1. For the various modes of ADAMP > 0, RATE_D serves the following purposes:

  - o **ADAMP = 1:** RATE_D sets the recovery rate for the damping factor θ in response to the progress in the Picard iteration; it also forms a limit on the response function to progress in the Picard iteration. Typical values for RATE_D, under this scenario, are 0.01 < RATE_D < 0.1. Under adaptive damping, if the user finds that the damping factor θ increases too rapidly, then reducing RATE_D will slow the rate of increase.

○ **ADAMP = 2:** Provided the Picard iteration is progressing satisfactorily, RATE_D adjusts the damping factor θ upward such that $\theta_j = \theta_{j-1} + RATE\_D \cdot \theta_{j-1}$, where *j* is the Picard iteration number. Typical values for RATE_D, under this scenario, are 0.01 < RATE_D < 0.1, although larger or smaller values may be used.

5. **Printout from the Solver**

- Enable progress reporting for the inner iteration (IPUNIT): If checked, a record of progress made by the Picard iteration for each time step is printed in the Run Listing file. This record includes the total number of dry cells at the end of each time step as well as the total number of PCG iterations necessary to obtain convergence.

3.8.1.2.6. Newton Solver (MODFLOW-NWT Only)

This package is activated only if the Upstream Weighting (UPW) Package is selected as the internal flow package, see Section 3.4.6 for details.

Figure 90 shows the dialog box for specifying the following required input parameters:

1. **Solution Options**

- **LINMETH:** This determines which matrix solver will be used.

- **OPTIONS:** This determines which default solver input values will be used. See table 2 of the MODFLOW-NWT user guide (Niswonger, et al., 2011) for the solver input values that will be used for the available options.

○ **SIMPLE (nearly linear model)** indicates that default solver input values will be defined that work well for nearly linear models. This would be used for models that do not include nonlinear stress packages, and models that are either confined or consist of a single unconfined layer that is thick enough to contain the water table within a single layer.

○ **MODERATE (moderately nonlinear model)** indicates that default solver input values will be defined that
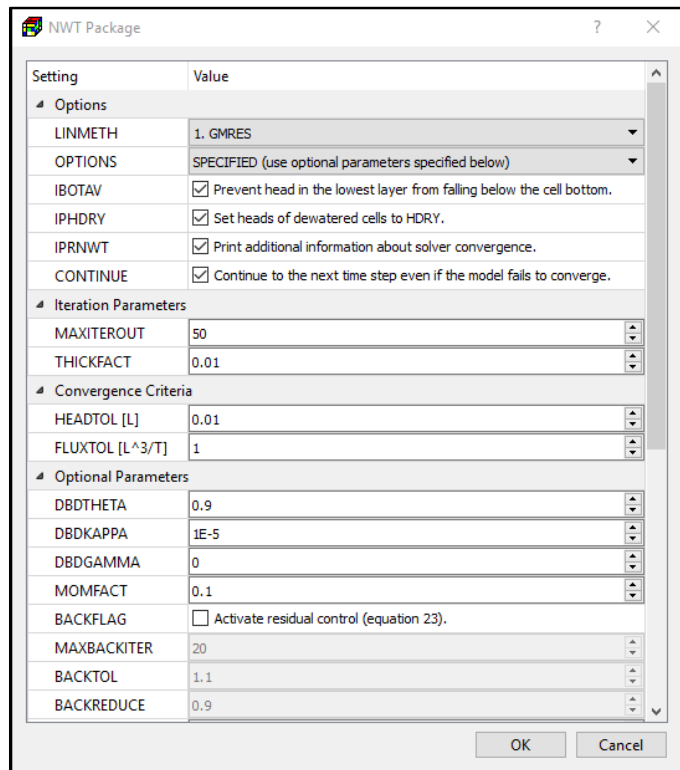
Figure 90. The NWT Package dialog box

work well for moderately nonlinear models. This would be used for models that include nonlinear stress packages, and models that consist of one or more unconfined layers. The MODERATE option should be used when the SIMPLE option does not result in successful convergence.

o **COMPLEX (highly nonlinear model)** indicates that default solver input values will be defined that work well for highly nonlinear models. This would be used for models that include nonlinear stress packages, and models that consist of one or more unconfined layers representing complex geology and surface water and groundwater interaction. The COMPLEX option should be used when the MODERATE option does not result in successful convergence.

o **SPECIFIED (use optional parameters specified below)** indicates that the optional solver input parameters will be specified in the Optional Parameters section of this dialog box.

- **IBOTAV** is a flag that indicates whether corrections will be made to groundwater head relative to the cell-bottom altitude if the cell is surrounded by dewatered cells. A correction will be made if this box is checked. This setting is problem specific and both checked and unchecked should be tested.

- **IPHDRY** is a flag that indicates whether groundwater head will be set to HDRY when the groundwater head is less than 1E-04 above the cell bottom.

- **IPRNWT** is a flag that indicates whether additional information about solver convergence will be printed to the run listing file.

- **CONTINUE:** Check this box to allow the model simulation to continue to the next step even if the model failed to converge.

2. **Iteration Parameters**

- **MAXITEROUT** is the maximum number of iterations to be allowed for solution of the outer (nonlinear) problem.

- **THICKFACT** is the portion of the cell thickness (length) used for smoothly adjusting storage and conductance coefficients to zero.

3. **Convergence Criteria**

- **Head Change (HEADTOL) [L]** is the maximum head change between outer iterations for solution of the nonlinear problem.

- **Residual (FLUXTOL) [L^{3}T^{-1}]** is the maximum root-mean-squared flux difference between outer iterations for solution of the nonlinear problem.

4. **Optional Parameters.** The optional parameters are used only if **OPTIONS** is set to **SPECIFIED**. See Table 2 of (Niswonger, et al., 2011) for a list of suggested values for these parameters.

- **DBDTHETA** is a coefficient, symbol θ in equation 21 of (Niswonger, et al., 2011), used to reduce the weight applied to the head change between nonlinear iterations

DBDTHETA is used to control oscillations in head. Values range between 0.0 and 1.0, and larger values increase the weight (decrease under-relaxation) applied to the head change.

- **DBDKAPPA** is a coefficient, symbol κ in equation 22 of (Niswonger, et al., 2011), used to increase the weight applied to the head change between nonlinear iterations. DBDKAPPA is used to control oscillations in head. Values range between 0.0 and 1.0, and larger values increase the weight applied to the head change.

- **DBDGAMMA** is a factor, symbol γ in equation 19 of (Niswonger, et al., 2011), used to weight the head change for iterations n–1 and n. Values range between 0.0 and 1.0, and greater values apply more weight to the head change calculated during iteration n.

- **MOMFACT** is the momentum coefficient m of equation 20 and ranges between 0.0 and 1.0. Greater values apply more weight to the head change for iteration n.

- **BACKFLAG** is a flag used to specify whether residual control will be used. A value of 1 indicates that residual control is active and a value of 0 indicates residual control is inactive.

- **MAXBACKITER** is the maximum number of reductions (backtracks) in the head change between nonlinear iterations. A value between 10 and 50 works well. **MAXBACKITER** is enabled and used only if **BACKFLAG** is checked.

- **BACKTOL** is the proportional decrease in the root-mean-squared error of the groundwater-flow equation used to determine if residual control is required at the end of a nonlinear iteration, as applied in equation 23 of (Niswonger, et al., 2011). **BACKTOL** is enabled and used only if **BACKFLAG** is checked.

- **BACKREDUCE** is a reduction factor, symbol B_r in equation 23 of (Niswonger, et al., 2011), used for residual control that reduces the head change between nonlinear iterations. Values should be between 0.0 and 1.0, where smaller values result in smaller head-change values. **BACKREDUCE** is enabled and used only if **BACKFLAG** is checked.

- The following parameters are enabled and used only if **LINMETH** is **1. GMRES**.

  o **MAXITINNER** is the maximum number of inner iterations for the linear solution.
  o **ILUMETHOD** is the method for incomplete factorization (ILU) used as a preconditioner.
  o **LEVFILL** is the fill limit for ILUMETHOD = 1 and is the level of fill for ILUMETHOD = 2. Recommended values: 5-10 for method 1, 0-2 for method 2.
  o **STOPTOL** is the tolerance for convergence of the linear solver. This is the residual of the linear equations scaled by the norm of the root mean squared error. Usually 10^{-8} to 10^{-12} works well.
  o **MSDR** is the number of iterations between restarts of the GMRES Solver.

- The following parameters are enabled and used only if **LINMETH** is "**2. χMD".**

  o **IACL** is the acceleration method.

  o **NORDER** is the scheme of ordering the unknowns.

  o **LEVEL** is the level of fill for incomplete LU factorization.

  o **NORTH** is the number of orthogonalization for the ORTHOMIN acceleration scheme. A number between 4 and 10 is appropriate. Small values require less storage, but more iterations may be required. This number should equal 2 for the other acceleration methods.

  o **IREDSYS** decides whether to apply reduced system preconditioning.

  o **RRCTOLS** is the residual reduction-convergence criteria.

  o **IDROPTOL** decides whether to use drop tolerance in the preconditioning.

  o **EPSRN** is the drop tolerance for preconditioning.

  o **HCLOSEXMD [L]** is the head closure criteria for inner (linear) iterations.

  o **MXITERXMD** is the maximum number of inner iterations for the linear solution.

3.8.1.3. Output Control

The primary output file of MODFLOW is the run listing file that can be found in *Models > Modflow > View > Run Listing File.* In addition to the run listing file, various simulation results can be saved
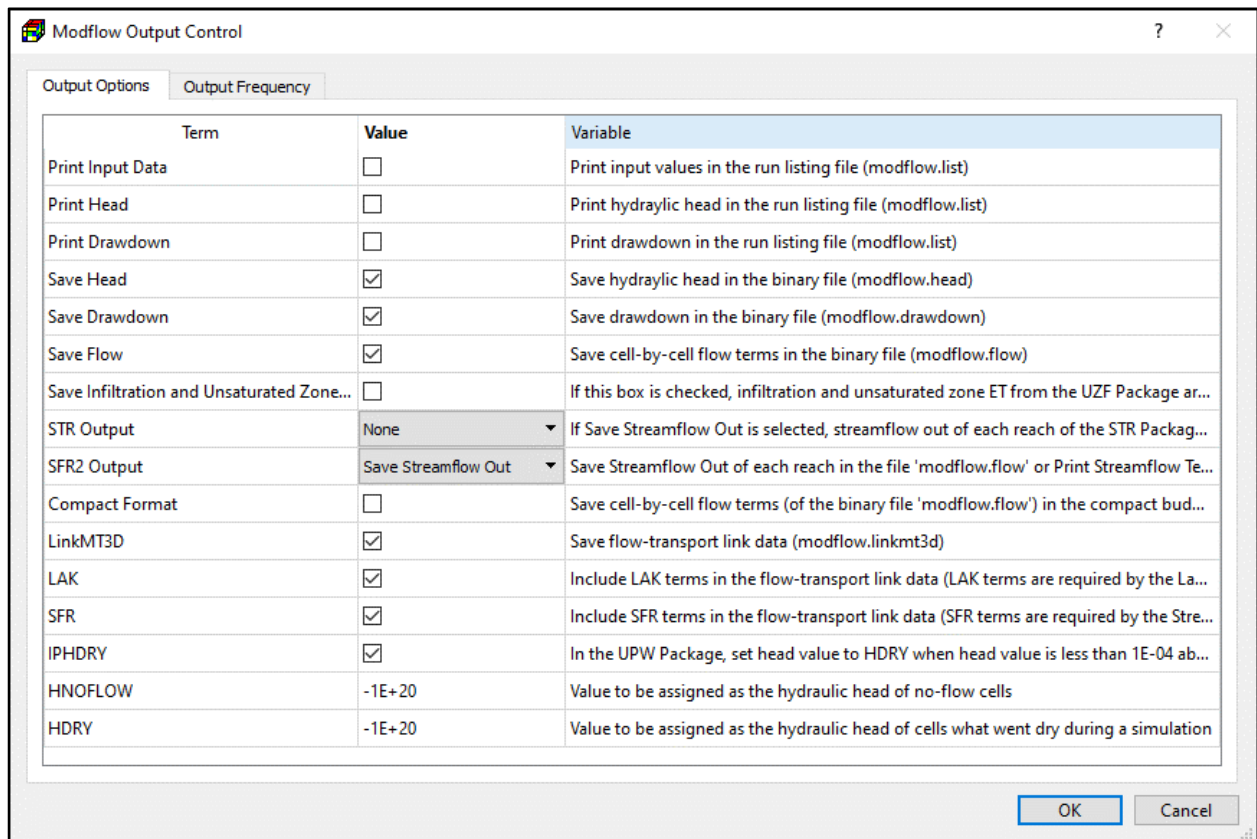
Figure 91. The Modflow Output Control dialog box

by checking the corresponding output terms in the Modflow Output Control dialog box (Figure 91). The available settings are described below.

1. **Output Options Tab**

   - **Print Input Data:** Check this box to write input values to the run listing file modflow.list.

   - **Print Head:** Hydraulic heads in individual model cells are the primary result of a MODFLOW simulation. Check this box to write the calculated hydraulic head values to the run listing file modflow.list.

   - **Print Drawdown:** Check this box to write the calculated drawdown values to the run listing file modflow.list.

   - **Save Head:** Check this box to save the calculated hydraulic head values in the binary file modflow.head.

   - **Save Drawdown:** Drawdown values in individual model cells are the differences between the initial hydraulic heads and the calculated hydraulic heads. If this box is checked, drawdown values are saved in the binary file modflow.drawdown.

   - **Save Flow:** If this box is checked, cell-by-cell flow terms are saved in the binary file modflow.flow. Cell-by-cell flow terms include stress flows (e.g., pumping), storage terms, constant-head flow terms, leakage (from/to river, drain, stream reaches, etc.), and flows across cell faces for individual cells.

   - **Save Infiltration and Unsaturated Zone ET:** If this box is checked, infiltration and unsaturated zone ET from the UZF Package are saved in the cell-by-cell flow file (modflow.flow.)

   - **STR Output:**
     o If Save Streamflow Out is selected, streamflow out of each reach of the STR Package will be saved in the binary file 'modflow.flow'.
     o If None is selected, streamflow out will not be saved.

   - **SFR2 Output:**
     o If Save Streamflow Out is selected, streamflow out of each reach will be saved in the file 'modflow.flow'.
     o If Print Streamflow Terms is selected, streamflow terms of each reach will be printed in the text file 'modflow.sfr2.list'. Streamflow terms include inflows, outflows, stream depth, width, streambed conductance, and head difference and gradient across the streambed.
     o If None is selected, neither streamflow out nor streamflow terms will be produced.

   - **Compact Format:** Check this box to save the cell-by-cell flow terms in a compact format. Note that existing software may not be compatible with this format. Note that

ZoneBudget may not work correctly, if the SFR2 Package is active and Save Streamflow Out (STR/SFR2) and Compact Format are both checked.

- **LinkMT3D**: if this box is checked, the flow-transport link data for MT3D will be saved in the binary file modflow.linkmt3d

- **LAK**[37]**:** If this box is checked, the flow terms associated with the LAK Package will be saved to the binary file modflow.linkmt3d. This option is required by the Lake Transport (LKT)Package of MT3D-USGS. If the LKT Package is not used, you may check or uncheck the *LAK* box.

- **SFR**[37]: if this box is checked, the flow terms associated with the SFR package (such as in-stream flow) will be saved to the binary file modflow.linkmt3d. This option is required by the Streamflow Transport (SFT) Package of MT3D-USGS. If the SFT Package is not used, you may check or uncheck the *SFR* box.

- **IPHDRY:** If the UPW Package (of MODFLOW-NWT) is used, activating this option will set the head value to HDRY when head have is less than 1E-04 above the cell bottom. Note that MODPATH works with MODFLOW-NWT provided that the IPHDRY is checked.

- **HNOFLOW:** This is the value to be assigned as the hydraulic head of no-flow cells.

- **HDRY:** This is the value to be assigned as the hydraulic head of cells what went dry during a simulation.

2. **Output Frequency Tab**

- **Stress Period** and **Time Step:** The simulation results of a time step are saved, if the stress period and the time step are even multiple of the respective specified value. If you intend to run a transport model, both values for Stress Period and Time Step should be set to 1.

- **Save the Result of the First Time Step of Each Stress Period:** if this box is checked, the results of the first time-step of each stress period are saved regardless of the specified values for Stress Period and Time Step.

- **Save the Result of the Last Time Step of Each Stress Period:** if this box is checked, the results of the last time step of each stress period are saved regardless of the specified values for Stress Period and Time Step.

---

[37] The executable of MODFLOW-2005 will not work if the SFR2 Package is activated and the *SFR* and/or LAK box is checked. If you need to use the SFT and/or the LKT Package, the respective *SFR* and/or LAK box must be checked and you must use MODFLOW-NWT for the flow simulation by either setting the UPW package as the internal flow package (Section 3.4.6) or assigning the executable of MODFLOW-NWT to the path of MODFLOW-2005 in the Preferences (Section 3.4.11) dialog box.

3.8.1.4. Run

Select this menu item to open the Run Modflow dialog box (Figure 92). The dialog box can be used to start the flow simulation with MODFLOW, to build input files to MODFLOW, or to check the model data. The available settings of the dialog box are described below.
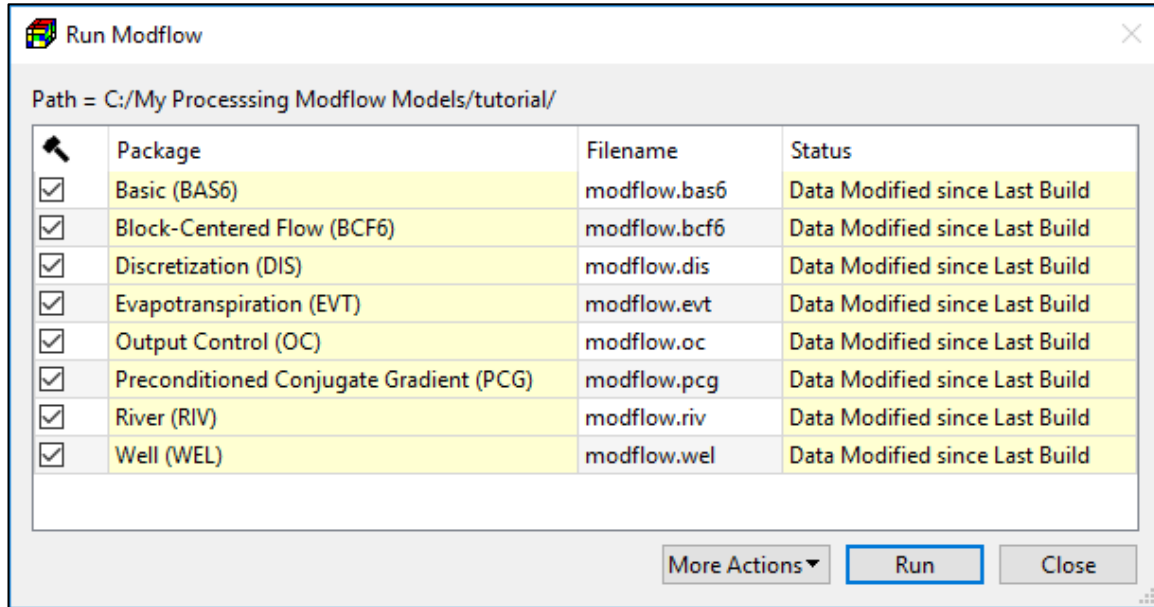
Figure 92. The Run Modflow dialog box

1. **Table**

   - 🔨 **The build box.** Prior to running a flow simulation, PM uses the user-specified data to build input files for MODFLOW. An input file will be built if its build box is checked. If an input file does not exist or the input data has been modified since the last build, its build box will be checked automatically.

   - **Package** is the name of the package of the flow model.

   - **Filename** is the name of the input file.

   - **Status** shows the status (such as Ready, Not Exist, etc.) of the input file.

2. **More Actions**

   - **Inspect Model Data:** Select this to check the geometry of the model and the consistency of the model data. Table 3 shows a list of items that are inspected by PM. The inspection report is saved in the *modflow_inspection_log.txt* file.

   - **Build Input Files:** Select this to build the input files with the checked build boxes. The name file modflow.nam and input file modflow.lmt for LMT8 package will also be built. The build log is stored in the *modflow_build_log.txt* file located in the model data folder.

- **Rebuild All Input Files:** Select this to rebuild all input files, except for existing read-only input files. The build log is stored in the *modflow_build_log.txt* file.

3. **Run:** Click this button to build input files with the checked build boxes and the start the flow simulation.

   - If LPF or BCF is selected as the internal flow package, the flow simulation will be carried out by the executable file of MODFLOW-2005 defined in the Preferences dialog box (Figure 26).

   - If UPW is selected as the internal flow package, the flow simulation will be carried out by the executable file of MODFLOW-NWT defined in the Preferences dialog box (Figure 26).

   The MODFLOW run progress will be displayed in the MODFLOW Output window. You may terminate the simulation at any time by clicking on the Terminate button.

Table 3. Model data inspected by PM

Inspected Items	Criteria
Initial head at constant-head cells	Initial head may not be lower than the cell bottom elevation.
Layer thickness	Thickness may not be zero or negative.
Top and bottom elevation of layers	Model layers may not overlap each other.
Horizontal hydraulic conductivity	Must be present and greater than zero if it is required.
Horizontal anisotropy	Must be present and greater than zero if it is required.
Vertical hydraulic conductivity	Must be present and greater than zero if it is required.
Vertical leakance	Must be present and greater than zero if it is required.
Vertical anisotropy	Must be present and greater than zero if it is required.
Specific storage	Must be present and greater than or equal to zero if it is required.
Specific yield	Must be present and greater than or equal to zero if it is required.
Storage coefficient	Must be present and greater than or equal to zero if it is required.
Transmissivity	Must be present and greater than zero if it is required.
Wetting threshold	Must be present if it is required.
Drain Package Drain with Return Flow Package	Drain conductance must be greater than zero. Drain cell must not be a constant-head cell. Drain cell should not be a no-flow cell. Drain elevation should not be lower than cell bottom elevation.
Flow and Head Boundary Package	Specified-flow cell should not be a constant-head cell. Specified-flow cell should not be a no-flow cell. Specified-head cell should not be a constant-head cell. Specified-head cell should not be a no-flow cell.
General-head boundary Package	GHB conductance must be greater than zero. GHB cell should not be a constant-head cell. GHB cell should not be a no-flow cell.
Lake Package	Lake cell must be a no-flow cell. Lake cell may not be a re-wettable cell. Lake cell may not be overlain by non-lake cells. Lakebed leakance must be greater than or equal to zero. Lake number should not be less than zero or greater than the total number of lakes.

Inspected Items	Criteria
Reservoir Package	Reservoir bed vertical hydraulic conductivity may not be negative. Reservoir bed thickness must be greater than zero.
River Package	Riverbed conductance must be greater than zero. RIV cell should not be a constant-head cell. RIV cell should not be a no-flow cell. River stage should not be lower than the riverbed bottom elevation.
Stream (STR) Package	Reach numbers within a segment must be consecutive. Streambed conductance of a STR cell must be greater than zero. STR cell must not be a constant-head cell. STR cell must not be a no-flow cell. Stream stage should not be lower than the streambed bottom elevation.
Streamflow-Routing (SFR2) Package	Reach numbers within a segment must be consecutive. SFR2 cell must not be a constant-head cell. SFR2 cell must not be a no-flow cell. Reach length of a SFR2 cell should be greater than zero. The following values are checked only if they are used in the simulation: Manning's roughness coefficient of a segment must be greater than zero. Depth1 and Depth2 of a segment must be greater than zero. Width1 and Width2 of a segment must be greater than zero. Streambed conductivity of a SFR2 cell must be greater than zero.
Time-variant specified head Package	CHD cell should not be a no-flow cell.
Well Package	WEL cell must not be a constant-head cell. WEL cell should not be a no-flow cell.

3.8.1.5. View

3.8.1.5.1. Run Listing File

Select this menu item to use the Text Editor (see Section 3.4.11) to display the run listing file modflow.list.

MODFLOW calculates a volumetric water budget for the entire model at the end of each time-step and save it in the run listing file. The volumetric water budget provides an indication of the overall acceptability of the numerical solution. In numerical solution techniques, the system of equations solved by a model consists of a flow continuity statement for each model cell. Continuity should therefore also exist for the total flows into and out of the entire model or a sub-region. This means that the difference between total inflow and total outflow should equal the total change in storage. The run listing file also contains other essential information. In case of difficulties in obtaining satisfactory model results, this supplementary information could be very helpful.

3.8.1.5.2. Model Inspection File

Select this menu item to use the Text Editor (see Section 3.4.11) to display the model inspection report file *modflow_check_log.txt.* See Section 3.8.1.4 and Table 3 for details about the model data that may be inspected by PM.

3.8.1.5.3. Scatter Chart

To display the scatter chart based on the head data, select *Scatter Chart > Head*. To display the scatter chart based on the drawdown data, select *Scatter Chart > Drawdown*. The Scatter Chart dialog box is shown in Figure 93.

1. **Chart**: The chart displays a scatter diagram using the simulated and observed data (see Data Tab below). The x-axis represents the observed values and the y-axis represents the calculated values. A linear least squares regression line can be displayed for each observation point if it has more than one data point. The regression line attempts to model the relationship between calculated and observed values by fitting the linear equation $y = m \cdot x + b$, where m is the slope of the line and b is the intercept of the line with the y-axis. Scatter diagrams are often used to present the goodness of fit of the observed data and the calculated data. If there is an exact agreement between measurement and simulation, all points lie on a 45° line with both the slope m and the coefficient of determination r^2 equal to 1. The values of m, b, and r^2 of each observation point can be displayed in the legend of the chart. In addition, the value of r^2 based on all displayed data points is displayed in the *Observation Points* tab (see below). Note that r^2 always equals to 1 if there are only two data points, since the linear regression would match the two data points perfectly. To interact with the chart, follow these steps:

   - When the mouse cursor is moved into the chart, it becomes a crosshair (+), and the approximate observed and calculated values are displayed next to the cursor.
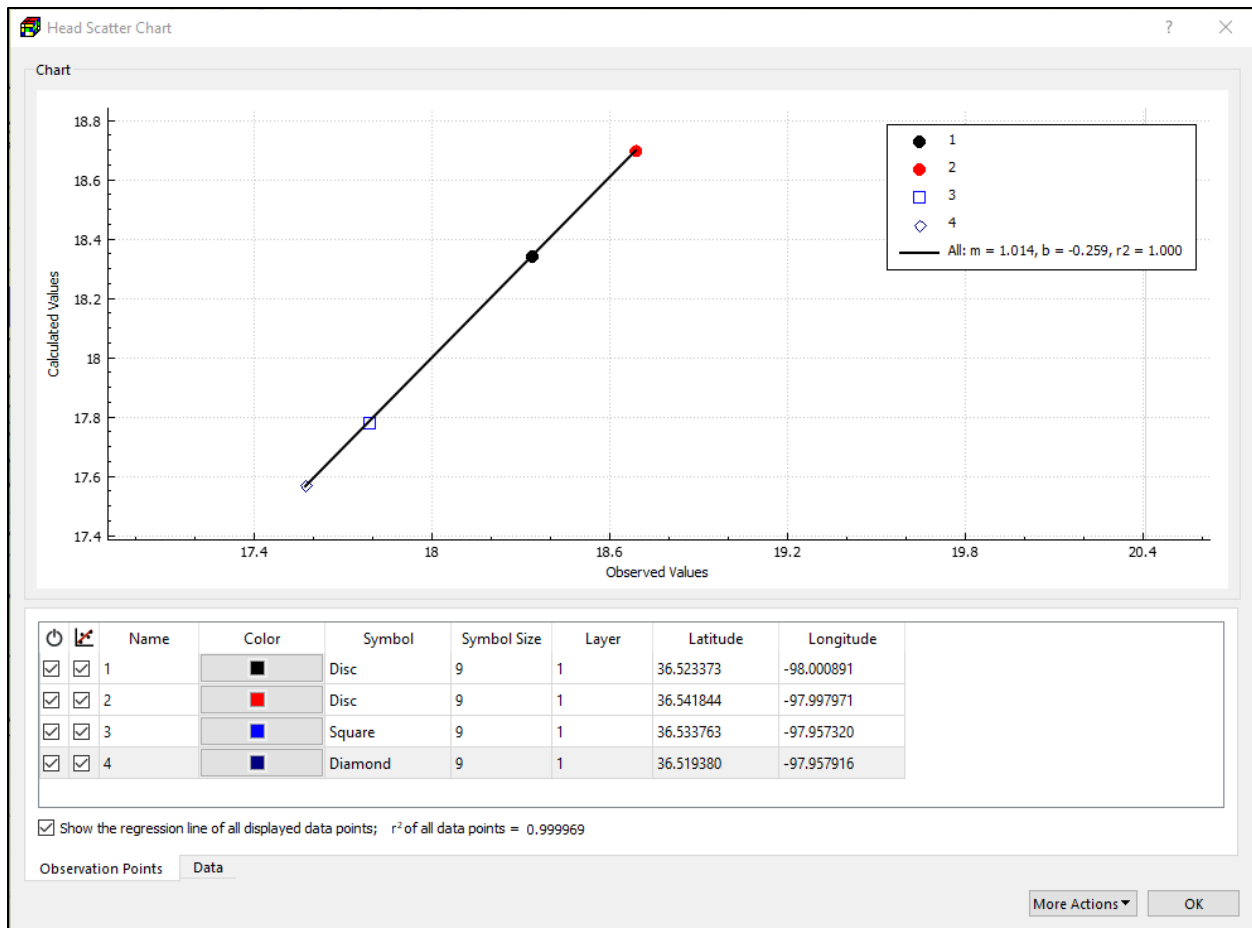
Figure 93. The Head Scatter Chart dialog box

- **To highlight a regression line**, click on it. The corresponding row in the Observation Points table will be highlighted. Alternatively, you can highlight the regression of an observation point by clicking on the respective Name field in the Observation Points table.

- **To pan around the chart**, press and hold the left mouse button and then move the mouse.

- **To zoom in/out on any part of the chart**, place the mouse cursor within the chart, scroll the mouse wheel forward or backward.

- **Popup Menu:** You can right-click on a chart to display the popup menu. The items in the popup menu are described below.

  o **Show Legend** or **Hide Legend**: This will show or hide the legend, which is displayed on the upper-right corner of the chart.

  o **Full Extent**: This will cause the display of the chart to zoom out to its data extent.

2. **Observation Points Tab:** This tab contains the observation points and their details. Each row in the table corresponds to an observation point. Observation points and observed values are defined by using the Observation Tool (Section 3.5.3).

- ⏻**:** Check/uncheck the box to turn on/off the display of the results in the chart. You may right-click on a row, and then select **Turn Off All But This** from a popup menu to switch off all other points.

- 📈**:** Check/uncheck the box to turn on/off the display of the regression line based on the data of the respective observation point.

- **Name** (read-only) displays the name of the observation point.

- **Label** (read-only) displays the label of the observation point.

- **Color** defines the color for the display of the symbol and regression line in the chart. Click on the **Color** header to assign a color to all points.

- **Symbol** defines the symbol for data points in the chart.

- **Symbol Size** defines the size of the symbol for data points in the chart.

- **Layer** (read-only) is the model layer where the observation point is located.

- **Latitude** and **Longitude** (read-only) are the coordinates of the observation point.

- **Display regression line of all data points:** Check/uncheck this box to turn on/off the display of the regression line based on the data all displayed data points.

- **r² of all data points:** This is the coefficient of determination based on all displayed data points.

3. **Data Tab:** This table contains the calculated and observed values. The columns of this table are as follows.

- **Observation Point** contains the names of the observation points.

- **Simulation Time** contains the simulation times that the calculated and observed values pertained to.

- **Date/Time** contains the calendar date/time (in UTC) that corresponds to the Simulation Time. The format of Date/Time corresponds to the ISO 8601 extended specification for representations of dates and times, taking the form YYYY-MM-DDTHH:mm:ssZ. Date/Time is only valid for years in the range 0 to 9999. Date/Time is blank for years beyond this range.

- **Calculated Value** contains the simulated head values at the respective observation points and simulation times. For a given simulation time t (at which the hydraulic heads or drawdown are saved in the binary file modflow.head or modflow.drawdown), the simulated value h_t at an observation point is obtained by using the following equation:

$$h_t = \sum_{i=1}^{4}(h_{i,t} \cdot A_i)/\sum_{i=1}^{4} A_i \qquad\qquad (40)$$

where

A_i are the areas as shown in Figure 94; for inactive cells $A_i = 0$

$h_{i,t}$ are the simulated head or drawdown values at the nodes surrounding the observation point for the simulation time t. Note that the nodes are in the same layer as the observation point.

Figure 94. Interpolation of simulated head values to an observation point

- **Observed Value** contains the observed values at the respective observation points and simulation times. The observed values are obtained by linear interpolating user-specified observed values to the respective simulation times.

4. **More Actions**

- **Activate:** Switch on the selected observation points[38].

- **Deactivate:** Switch off the selected observation points[38].

- **Save Chart**: Select this item to display the Save Image dialog box that allows you to save the chart as in a support image format (JPEG, PNG, or BMP) or in the PDF format.

- **Save Data**: Select this item to display the Save Data dialog box that allows you to save the content of the Data table in the following file types

  o **Comma Delimited (*.csv)**: All values of the data table are exported to a comma delimited text file.

  o **Excel Workbook (*.xlsx)**: This workbook contains several tabs. The first tab contains the observation points. The other tabs contain the observed and calculated data of individual observation points.

  o **Excel Workbook [Calculated Values Only] (*.xlsx)**: This workbook contains two tabs. The first tab contains the observation points. The second tab contains the calculated values at the observation points.

  o **Excel Workbook [Condensed Format] (*.xlsx)**: This workbook contains two tabs. The first tab contains the observation points. The second tab contains the time-series of calculated and observed values at the observation points.

- **Print Chart:** Select this item to open the Print dialog box that enables you to print the chart.

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[38] You may select multiple rows from the Observation Point table by using combinations of Ctrl-click and Shift-click.
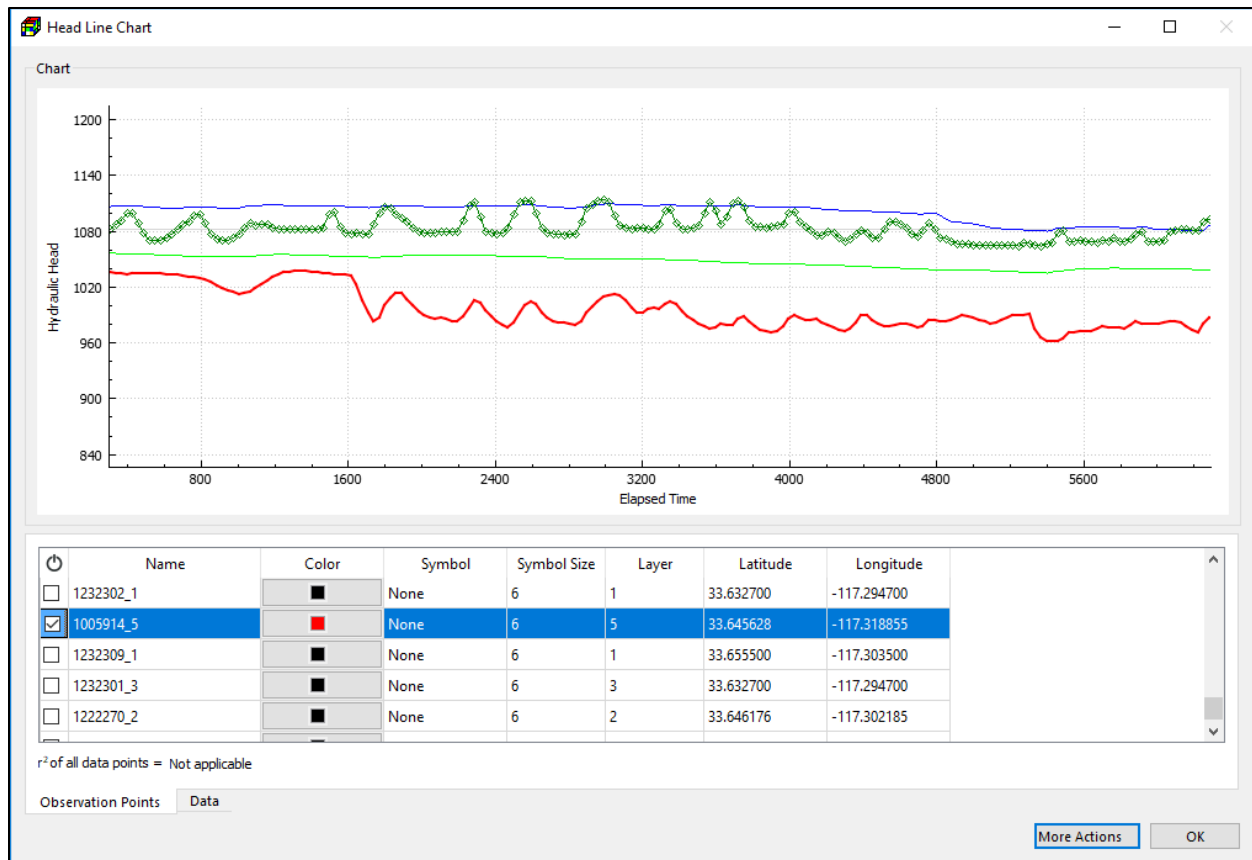
Figure 95. The Head Line Chart dialog box

3.8.1.5.4. Line Chart

To display the line chart based on the head data, select *Line Chart > Head*. To display the line chart based on the drawdown data, select *Line Chart > Drawdown*. The Line Chart dialog box is shown in Figure 95.

1. **Chart**: The chart displays a line graph using the simulated and observed data (see Data tab below). The x-axis represents the simulation time and the y-axis represents the calculated and observed data. Two time-series curves are displayed for each observation point. Calculated and observed data points are represented by graphic symbols. Solid lines connect the calculated data and dashed lines connect the observed data. To interact with the chart, follow these steps:

   - When the mouse cursor is moved into the chart, it becomes a crosshair (+), and the head (or drawdown) value, simulation time, and corresponding calendar date/time are displayed next to the cursor.

   - **To pan around the chart**, move the mouse cursor into the chart, press and hold the left mouse button, and then move the mouse.

   - **To zoom in/out on any part of the chart**, place the mouse cursor within the chart, scroll the mouse wheel forward or backward.

- **You can limit the zoom and pan** to the x or y direction by selecting the x or y-axis first. An axis is selected by clicking on it. A selected axis is colored in blue. To deselect an axis, simply click on any part of the respective chart.

- **To highlight the time-series curves of an observation point**, click on a curve or a data point symbol. The corresponding row in the Observation Points table will be highlighted. Alternatively, you can highlight the time-series curves of an observation point by clicking on the respective Name field in the Observation Points table.

- **Popup Menu:** You can right-click on a chart to display the popup menu. The items in the popup menu are described below.

   o **Full Extent**: This will cause the display of the chart to zoom out to its data extent.

   o **Show Legend** or **Hide Legend**: This will show or hide the legend, which is displayed on the upper-right corner of the chart.

   o **Use Logarithmic Scale** or **Use Linear Scale:** This allows you to switch the y-axis between logarithmic and linear scales. This option is only available when all calculated and observed values are greater than zero.

2. **Observation Points Tab:** This tab contains the observation points and their details. Each row in the table corresponds to an observation point. Observation points and observed values are defined by using the Observation Tool (Section 3.5.3).

- ⏻: Check/uncheck the box to turn on/off the display of the results in the chart.

- **Name** (read-only) displays the name of the observation point.

- **Label** (read-only) displays the label of the observation point.

- **Color** defines the color for the display of the symbol and time-series curves in the chart.

- **Symbol** defines the symbol for data points in the chart.

- **Symbol Size** defines the size of the symbol for data points in the chart.

- **Layer** (read-only) is the model layer where the observation point is located.

- **Latitude** and **Longitude** (read-only) are the coordinates of the observation point.

- **r² of all data points:** This is the coefficient of determination based on all calculated and observed data pairs of observation points that are turned on. Note that r^2 always equals to 1 if there are only two data points.

3. **Data Tab:** This table contains the calculated and observed values. The contents of this table are the same as those of the Scatter Chart dialog box. See the previous section for details.

4. **More Actions:** The functionalities of this menu are the same as those of the Scatter Chart dialog box. See the previous section for details.

3.8.1.5.5. Volume Summary

Select this menu item to calculate the amount of water in the model based on the starting hydraulic head, the simulated hydraulic head (stored in the modflow.head file), layer types (unconfined, confined, or convertible), layer geometry (top and bottom elevation of layers), and aquifer parameters (S, Ss, and Sy). If aquifer parameters are not specified, the respective default values are used for the calculation.

The calculated results are stored in a comma-separated value file consisting of a number of records. Each record represents storage terms in each time step and layer. A record includes the following terms.

- **SimulationTime** is the simulation time.

- **Period** is the stress period. The records with Period = 0 represent the initial condition based on the starting hydraulic head.

- **TimeStep** is the time step within the given Period.

- **Date** is the calendar date in the form of year-month-day. The date corresponds to the given Period and TimeStep.

- **Layer** is the model layer.

- **Vs** [L^3] is the volume of water stored due to compressibility (based on S or Ss) of the given date and layer. The volume of water stored in a cell due to compressibility (vs) is calculated based on the following rules.

    o For confined/convertible layers:

    $$vs = (t - b) \times Area \times S_s \times (h - z) \qquad if\ h \geq t$$
    $$vs = (h - b) \times Area \times S_s \times ((h - b)/2) \qquad if\ b < h < t$$
    $$vs = 0 \qquad if\ h \leq b$$

    Where

    S_s [L^{-1}] is the specific storage of the cell,

    h [L] is the hydraulic head in the cell,

    z [L] is the elevation of the center of the cell,

    t [L] is the elevation of the top of the cell, and

    b [L] is the elevation of the bottom of the cell, and

    $Area$ [L^2] is the area of the cell,

    $(h - b)$ is the saturated thickness of the cell when it is not under confined condition, and

$(h - b)/2$ represents the average hydraulic head that acts on the water within the cell when it is not under confined condition.

- o For unconfined layers:

$$vs = (h - b) \times Area \times S_s \times ((h - b)/2) \quad if\ h > b$$
$$vs = 0 \qquad\qquad\qquad\qquad\qquad\qquad if\ h \le b$$

- **Vsy** [L³] is the amount of water stored in the pore space (based on Sy) of the given date and layer. The amount of water stored in the pore space of a cell (vsy) is calculated based on the following rules.

- o For confined/convertible layers:

$$vsy = (t - b) \times Area \times S_y \qquad if\ h \ge t$$
$$vsy = (h - b) \times Area \times S_y \qquad if\ b < h < t$$
$$vsy = 0 \qquad\qquad\qquad\qquad\qquad if\ h \le b$$

Where

S_y [-] is the specific yield of the cell.

- o For unconfined layers:

$$vsy = (h - b) \times Area \times S_y \qquad if\ h > b$$
$$vsy = 0 \qquad\qquad\qquad\qquad\qquad if\ h \le b$$

- **Volume** [L³] is the total amount of water of the model at the given date. The value is only calculated for the record with **Layer** equals to the bottom layer of the model.

3.8.2. ZoneBudget

There are situations in which it is useful to calculate flow terms for various zones (i.e., subregions) within the model domain. To facilitate such calculations, MODFLOW saves the computed flow terms for individual cells in the modflow.flow file (also known as the cell-by-cell budget file). The computed flow terms include (1) inflows or outflows due to external stresses or boundaries, such as pumping well, recharge, or general-head boundary; (2) storage changes; (3) flows from or to constant-head boundary; and (4) flows across cell faces.

Zonebudget (Harbaugh, 1990) is a program that reads flow terms from the cell-by-cell budget file and produces water budgets for user-defined zones within the model domain. The zones are defined by assigning zone numbers to model cells. Follow the steps below to compute water budgets with ZoneBudget.

1. **Define Zone Numbers** with the Data Editor by selecting *Models > ZoneBudget > Zones.*
   - If zone numbers are not defined, the entire model will be treated as a single zone, with the zone number set to 1.

- Zone numbers from 0 to 999 are allowed. The number 0 indicates that a cell is not associated with any zone and will be excluded from the zone budget calculation.

2. **Run the ZoneBudget program** by selecting *Models > ZoneBudget > Run*.

   - PM will build the input file to the ZoneBudget and then start the ZoneBudget program.

   - The run progress of ZoneBudget will be displayed in the ZoneBudget Output window. You may terminate the simulation at any time by clicking on the Terminate button. Once the calculation is complete, you can click the Close button to close the window.

3. **Review the results:**

   - **Models > ZoneBudget > View > Listing File:** This listing file contains the water budget of all zones of individual time steps at which flow terms are saved in the budget file.

   - **Models > ZoneBudget > View > CSV File:** For each time, for which the flow terms are saved in the budget file, there is one line for each in-flow term and each out-flow term along with totals. The zones are displayed in columns, so one table displays all zones. This makes it easy to compare any budget term for all the different zones. The CSV file is formatted in the way suitable to be loaded into a spreadsheet application.

   - **Models > ZoneBudget > View > CSV2 File[39]:** The CSV2 file displays the complete budget for one zone and one time in a single line. Each column has a separate inflow or outflow budget term. The rows can be sorted by time within the spreadsheet program, which makes it possible to easily see how each term changes with time. The CSV2 file is formatted in the way suitable to be loaded into a spreadsheet application.

3.8.3. MT3D/SEAWAT

This menu provides the interface to MT3D-USGS (Bedekar, et al., 2016) and SEAWAT (Langevin, et al., 2007). The former simulates transport processes based on the flow results of MODFLOW, thus a MODFLOW run must be completed prior to using MT3D-USGS. SEAWAT couples the flow and transport processes, therefore does not require a separate MODFLOW run.

3.8.3.1. Settings

The first step to use MT3D or SEAWAT is to define the species, packages, and the reaction type in the Transport Settings dialog box (Figure 96). The features of this dialog box are detailed below.

1. **More Actions**

   - **Import MT3D Model:** Select this option to import a transport model saved in the MT3D-USGS (Bedekar, et al., 2016) or MT3DMS (Zheng, et al., 1999) format. After selecting this option, you will need to (1) select the name file of the MODFLOW model, and then (2) select the name file of the MT3D model. The grid size of the selected

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[39] At the time of writing, *if a package (such as general-head boundary) is active in the flow model, but no cells are defined for that package in a stress period, the inflow and outflow budget term of that package will be excluded for that stress period, leading to an incorrectly formatted CSV2 file.*
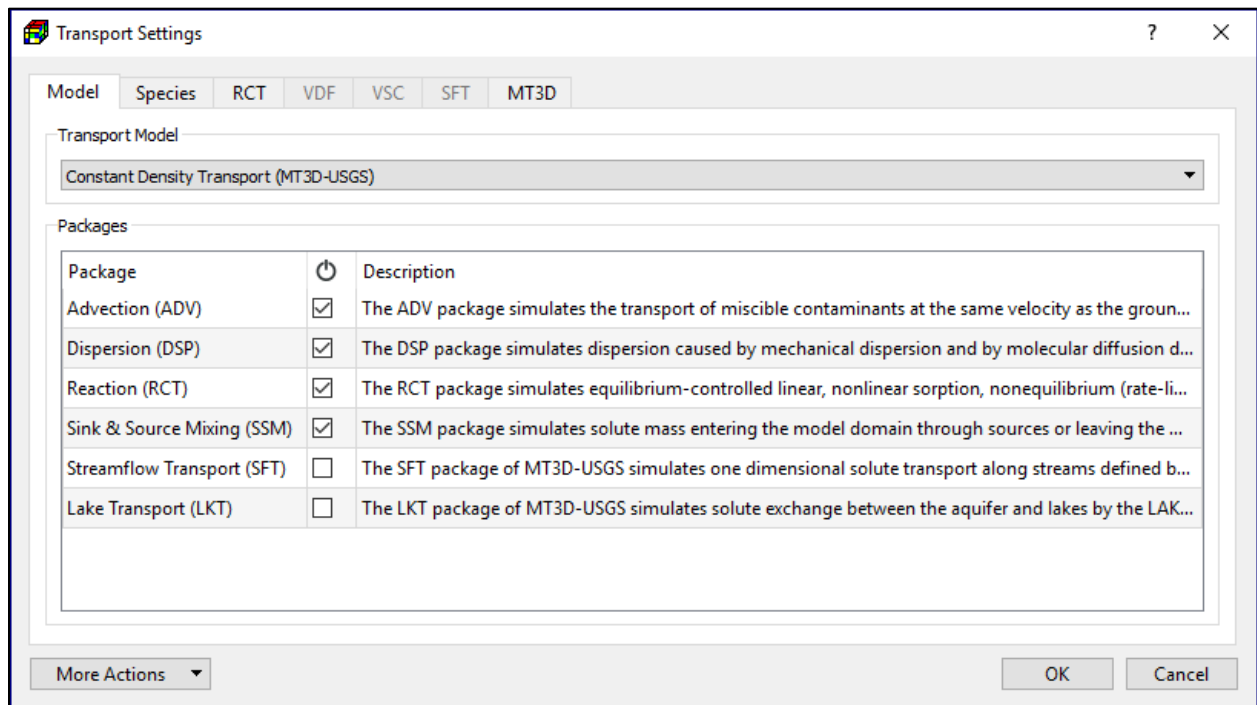
Figure 96. The Model tab of the Transport Settings dialog box

MODFLOW and MT3D models must be identical. All packages of MT3D listed in Section 5.2.2.1 may be imported.

- **Import SEAWAT Model:** Select this option to import a transport model saved in the SEAWAT (Langevin, et al., 2007) format. All packages of MT3D and SEAWAT listed in Sections 5.2.2.1 and 5.2.3.1 may be imported.

2. **Model Tab** (Figure 96) defines the transport model and packages to be used in the simulation.

- **Transport Model** contains the following items:

  o **Constant Density Transport (MT3D-USGS):** If this item is selected, the transport simulation will be carried out by the executable file of MT3D-USGS defined in the Preferences dialog box (Figure 26). The transport process will be density-independent.

  o **Constant Density Transport (MT3DMS):** If this item is selected, the transport simulation will be carried out by the executable file of MT3DMS defined in the Preferences dialog box (Figure 26). The transport process will be density-independent.

  o **Variable Density Flow and Transport (SEAWAT):** If this item is selected, the transport simulation will be carried out the executable file of SEAWAT defined in the Preferences dialog box (Figure 26). The transport process can be density-dependent.

- **Packages:** The table contains the available packages of the selected transport model. Check/uncheck the boxes in the ⏻ column to turn on/off packages.

  o **Advection (ADV)**: The ADV package simulates the transport of miscible contaminants at the same velocity as the groundwater.

  o **Dispersion (DSP):** The DSP package simulates dispersion caused by mechanical dispersion and by molecular diffusion driven by concentration gradients.

  o **Reaction (RCT):** The RCT package simulates equilibrium-controlled linear, nonlinear sorption, nonequilibrium (rate-limited) sorption, and kinetic reactions.

  o **Sink & Source Mixing (SSM):** The SSM package simulates solute mass entering the model domain through sources or leaving the model domain through sinks.

  o **Streamflow Transport (SFT):** The SFT package of MT3D-USGS simulates one dimensional solute transport in the stream network that is defined by the SFR2 package. If this package is activated, it is required to use MODFLOW-NWT for the flow simulation[35, 40]. You must set the UPW package as the internal flow package (Section 3.4.6) or assign the executable of MODFLOW-NWT to the path of MODFLOW-2005 in Preferences (Section 3.4.11).

  o **Lake Transport (LKT):** The Lake Transport (LKT) Package calculates solute concentrations in lakes. The package uses simulated flows calculated by the Lake (LAK3) Package of MODFLOW. Solute entering the lake is instantaneously mixed throughout the entire volume of the lake while the constituent concentration in lake seepage is equal to the concentration in the lake.

  o **Variable-Density Flow (VDF):** The VDF Process of SEAWAT solves the variable-density ground-water flow equation. Activate this package to include the density effect in the simulation.

  o **Viscosity (VSC):** The VSC package of SEAWAT simulates effects of viscosity variations that are implemented in the LPF package[41].

3. **Species Tab** (Figure 97) defines the species to be used in the simulation. The table contains the species and related parameters.

   - ⏻: Check/uncheck the boxes in this column to activate/deactivate species.

   - **Species Name:** Name of the species.

   - **Yield:** The value of the yield coefficient between the current species and the next species. This is used only if the first-order chain reaction is simulated.

   - **Density:** This is used only if the Variable Density Flow (VDF) process of SEAWAT is turned on. If the Density box of a species is checked, the concentration of that species will affect the fluid density (see DRHODC below). If all Density boxes are cleared,

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[40] MODFLOW-NWT is required as the current version of MODFLOW-2005 is not compatible with the SFT Package.
[41] The effects of viscosity variations are implemented only for the Layer-Property Flow (LPF) Package; the Block-Centered Flow (BCF) and Upstream-Weighting (UPW) Packages cannot be used with the VSC Package.
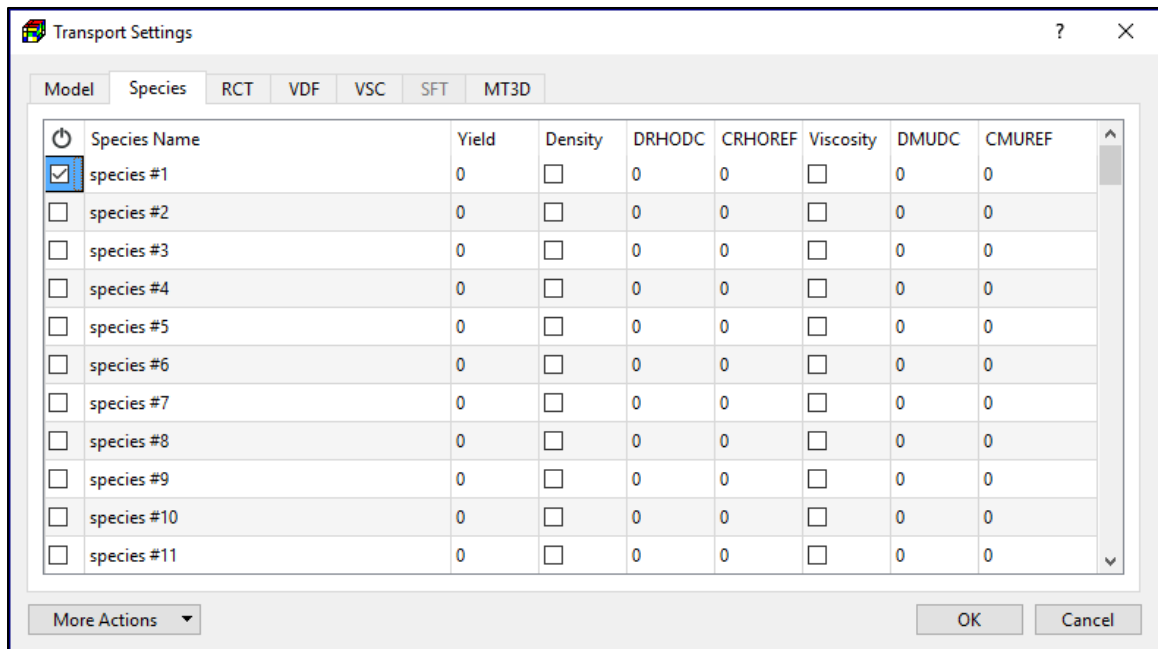
Figure 97. The Species Tab of the Transport Settings dialog box

SEAWAT runs in the uncoupled mode and you must specify the fluid density (see Section 3.8.3.3.5) and has the option to determine the density of the source fluid using WELDENS, RIVDEN and GHBDENS in the VDF Tab.

- **DRHODC** is the slope that relates fluid density (ρ) to solute concentration (C), i.e., $\partial\rho/\partial C$. This is used only if the Variable Density Flow (VDF) process of SEAWAT is turned on.

- **CRHOREF** is the reference concentration (i.e., C0) for the species. For most simulations, CRHOREF should be specified as zero. This is used only if the Variable Density Flow (VDF) process of SEAWAT is turned on.

- **Viscosity:** This is used only if the Viscosity (VSC) package of SEAWAT is turned on. If the Viscosity box of a species is checked, the concentration of that species will affect the fluid viscosity (see DMUDC below). If all Viscosity boxes are cleared, you must specify the viscosity value (see Section 3.8.3.3.6).

- **DMUDC** is the slope that relates dynamic viscosity (μ) to solute concentration (C), i.e., $\partial\mu/\partial C$. This is used only if the Viscosity (VSC) package of SEAWAT is turned on.

- **CMUREF** is the reference concentration for the species. This is used only if the Viscosity (VSC) package of SEAWAT is turned on.

4. **RCT Tab** (Figure 98) contains options for the Reaction Package. The available sorption and reaction types and their required parameters are described as follows. The required parameters for the selected options must be specified in the *Models > MT3D/SEAWAT > Packages > Reaction (RCT)* menu.
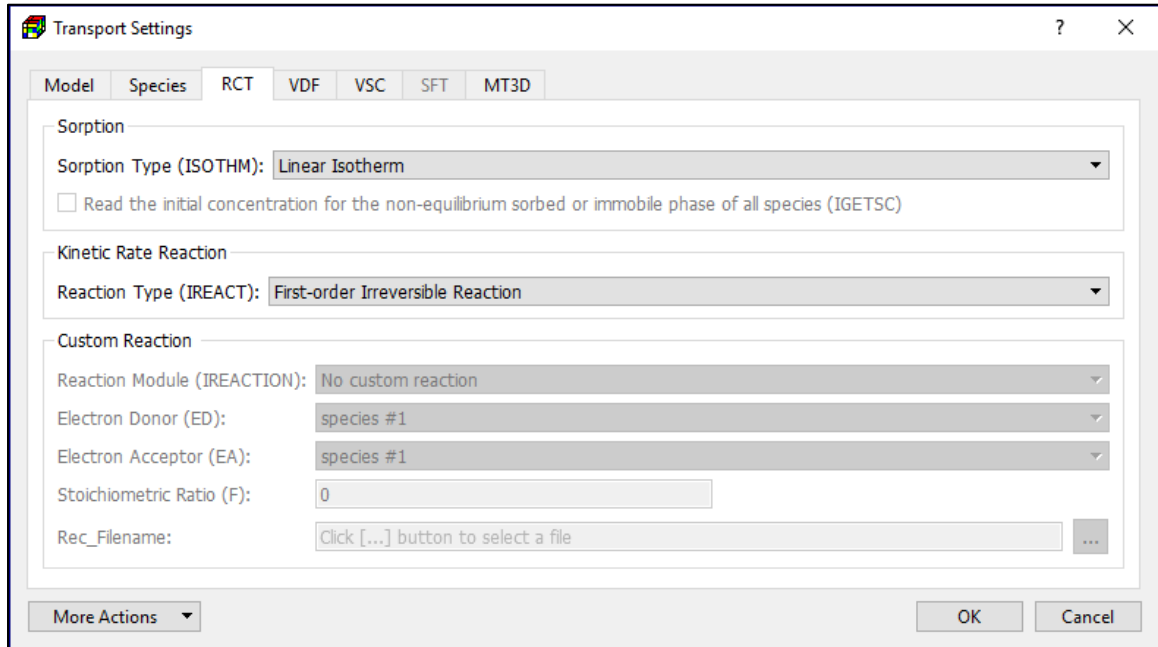
Figure 98. The RCT tab of the Transport Settings dialog box

- **Sorption:**
  - **Sorption Type** defines the type of sorption or dual-domain transfer. Equilibrium-controlled sorption isotherms are implemented in MT3D through use of the retardation factor R.
    - **No sorption**: Sorption is not simulated.
    - **Linear Isotherm** simulates linear equilibrium sorption and assumes that the sorbed concentration $\bar{C}$ is directly proportional to the dissolved concentration C. The retardation factor R is therefore independent of the concentration values and is calculated only once for each cell at the beginning of the simulation.

$$\bar{C} = K_d \cdot C \tag{41}$$

$$R = 1 + \frac{\rho_b}{n} \cdot K_d \tag{42}$$

where n [-] is the porosity of the porous medium in a cell; K_d [L^{3}M^{-1}] is the distribution coefficient that depends on the solute species, nature of the porous medium, and other conditions of the system; and ρ_b [ML^{-3}] is the bulk density of the porous medium of the cell.

- **Freundlich Isotherm** simulates nonlinear equilibrium sorption with the following equation.

$$\overline{C} = K_f \cdot C^a \tag{43}$$

The retardation factor at the beginning of a transport step is calculated by

$$R = 1 + \frac{\rho_b}{n} \cdot a \cdot C^{a-1} \cdot K_f \tag{44}$$

Where C is the solute concentration in a cell at the beginning of a transport step; a [-] is the Freundlich exponent; and K_f [L^3M^{-1}] is the Freundlich constant.

- **Langmuir Isotherm** simulates nonlinear equilibrium sorption with the following equation.

$$\overline{C} = (K_L \cdot \overline{S} \cdot C)/(1 + K_L \cdot C) \tag{45}$$

The retardation factor at the beginning of a transport step is calculated by

$$R = 1 + \frac{\rho_b}{n} \cdot \frac{K_L \cdot \overline{S}}{(1 + K_L \cdot C)^2} \tag{46}$$

where K_L [L^3M^{-1}] is the Langmuir constant and $\overline{S}$ [MM^{-1}] is the sorption capacity of the porous medium.

- **First-order Kinetic Sorption** simulates nonequilibrium sorption. It is assumed that sorption can be represented by a first-order reversible kinetic sorption defined by

$$\rho_b \cdot \frac{\partial \overline{C}}{\partial t} = \beta \cdot \left(C - \frac{\overline{C}}{K_d} \right) \tag{47}$$

Where β [T^{-1}] is the first-order mass transfer rate between the dissolved and sorbed phases.

- Dual-Domain Mass Transfer (without Sorption), Dual-Domain Mass Transfer (with Sorption), and Dual-Domain Mass Transfer (with Different Sorption Coefficients in Mobile and Immobile Domains): Dual-domain means that two kinds of continuum, e.g. a fractured medium and the porous medium, exist simultaneously in the same spatial region, i.e., the same model cells. In fractured aquifers, water moves faster along fractures than it does in a rock formation and the solute transport is often controlled by advection along the fractures and dominated by dispersion in the porous block along the fractures.

MT3D uses the dual-domain concept to approach extremely heterogeneous porous media or media composed of fractures and pores. In this approach, the effective porosity is used as the primary porosity for the pore spaces filled with mobile water (i.e., fractures) and the secondary porosity for the pore spaces

filled with immobile water (i.e., rock formation) is defined separately. The sum of the primary and the secondary porosities is the total porosity of the medium.

The sorption process in the mobile and immobile domain is simulated by using the linear isotherm.

The exchange of the dissolved mass between the mobile and immobile domains can be defined by

$$n_{im} \cdot \frac{\partial C_{im}}{\partial t} = \zeta \cdot (C_m - C_{im}) \tag{48}$$

where n_{im} [-] is the porosity of the immobile domain; C_{im} [ML^{-3}] is the solute concentration in the immobile domain; C_m [ML^{-3}] is the solute concentration in the mobile domain; and ζ [T-1] is the first-order mass transfer rate between the mobile and immobile domains. As the mass transfer rate ζ increases, the dual-domain model functions more and more like the single-domain model with a porosity approaching the total porosity of the porous medium.

o **IGETSC** is a flag indicating whether the initial concentration for the non-equilibrium sorbed or immobile phase of all species should be read when first-order kinetic sorption or dual-domain mass transfer is simulated.

  – If this box is checked, the initial concentration for the sorbed phase or immobile liquid phase of all species will be used in the simulation.
  – If this box is unchecked, the initial concentration for the sorbed or immobile phase is not used. The sorbed phase is assumed to be in equilibrium with the dissolved phase and the immobile domain is assumed to have zero concentration.

• **Kinetic Rate Reaction** defines the type of kinetic rate reaction. Note that *first-order irreversible reaction* and *MONOD kinetic reaction* are not intended for modeling chemical reactions between species.

  o **No Kinetic Rate Reaction**: kinetic rate reaction is not simulated.
  o **Zero-order Reaction:** The reaction rate of a zero-order reaction is constant and independent of the concentration of reacting substances. In MT3D, the zero-order reaction rate coefficients for the dissolved phase (in [ML^{-3}T^{-1}]) and sorbed phase (in [MM^{-1}T^{-1}]) may be specified separately. The convention for both coefficients are positive values for decay and negative values for production.
  o **First-order Irreversible Reaction:** The concentration change due to the chemical reaction from one transport step to another at a cell can be expressed as

$$\Delta C = -\frac{\Delta t}{R} \cdot \left[\lambda_1 \cdot C + \lambda_2 \cdot \frac{\rho_b}{n} \cdot \bar{C} \right] \tag{49}$$

where λ_1 [T⁻¹] is the first-order rate for the dissolved phase; λ_2 [T⁻¹] is the first-order rate for the sorbed phase; Δt is the transport time-step; and $\bar{C}$ is the mass of the solute species adsorbed on the solids per unit bulk dry mass of the porous medium at the beginning of each transport step. $\bar{C}$ is in equilibrium with solute concentration C in the cell.

The rate constant λ is usually given in terms of the half-life. Generally, if the reaction is radioactive decay, λ_2 should be set equal to λ_1. However, for certain types of biodegradation, λ_2 may be different.

o **First-order Chain Reaction**: The first-order chain reaction is implemented in MT3D for both dissolved and sorbed phases. Considering the dissolved phase, the changes in the concentration values of involved species within a transport time-step are calculated in the following sequential order:

$$\frac{\Delta C^1}{\Delta t} = -\lambda^1 \cdot C^1$$
$$\frac{\Delta C^2}{\Delta t} = -\lambda^2 \cdot C^2 + Y_{1/2} \cdot \lambda^1 \cdot C^1 \qquad\qquad (50)$$
$$...$$
$$\frac{\Delta C^k}{\Delta t} = -\lambda^k \cdot C^k + Y_{k-1/k} \cdot \lambda^{k-1} \cdot C^{k-1}$$

where λ^k specifies the first-order reaction coefficient for species k and $Y_{k-1/k}$ sets the yield coefficient between species k-1 and k. Yield coefficients are based on stoichiometric relations between the species for which relations are specified.

o **Monod Kinetic Reaction:** The concentration change due to the chemical reaction from one transport step to another at a cell can be expressed by

$$\Delta C = -Mic_t \cdot \mu_{max} \cdot \frac{C}{K_s + C} \qquad\qquad (51)$$

where

Mic_t is the total microbial concentration [ML⁻³] at the cell,

K_s is a constant, described by (Alexander, 1999), called the half-saturation constant, and is equal to the constituent concentration [ML⁻³] at which the microbial growth rate is half of μ_{max}. It is important to note that the microbial concentration depends on many chemical and biological considerations and is therefore difficult to estimate. The total microbial concentration is assumed constant in MT3D. The values of $Mic_t \cdot \mu_{max}$ and K_s must be specified by the user and need to be carefully considered during model calibration procedures. The Monod kinetics are available only for dissolved-phase organic compounds and do not consider sorbed concentrations, though reduction in dissolved concentrations resulting from microbial remediation may lead to desorption and a consequent rebound of concentration.

- **Custom Reaction:** See the input instruction of the MT3D-USGS software distribution (Bedekar, et al., 2016) for details about custom reaction modules.

  - **Reaction Module (IREACTION)** defines the custom reaction module. At least two species must be simulated when a custom reaction module is used.
  - **Electron Donor (ED)** is the electron donor in the EA/ED reaction.
  - **Electron Acceptor (EA)** is the electron acceptor in the EA/ED reaction.
  - **Stoichiometric ratio (F):** F is used in the simulated equation as follows: ED + F × EA → Product.
  - **Rec_Filename:** This is the file that stores parameters required for simulating a user-defined kinetic reaction.

5. **VDF Tab** (Figure 99) contains options for the Variable-Density Flow Process of SEAWAT.

   - **IWTABLE:** Check the box to activate the variable-density water-table correction. For details, see Equation 82 of (Guo, et al., 2002).

   - **MFNADVFD** this defines the method for calculating Internodal density values.

   - **NSWTCPL** is used to determine the flow and transport coupling procedure.

     - If NSWTCPL = 0 or 1, flow and transport will be explicitly coupled using a one-timestep lag. The explicit coupling option is normally much faster than the iterative option and is recommended for most applications.
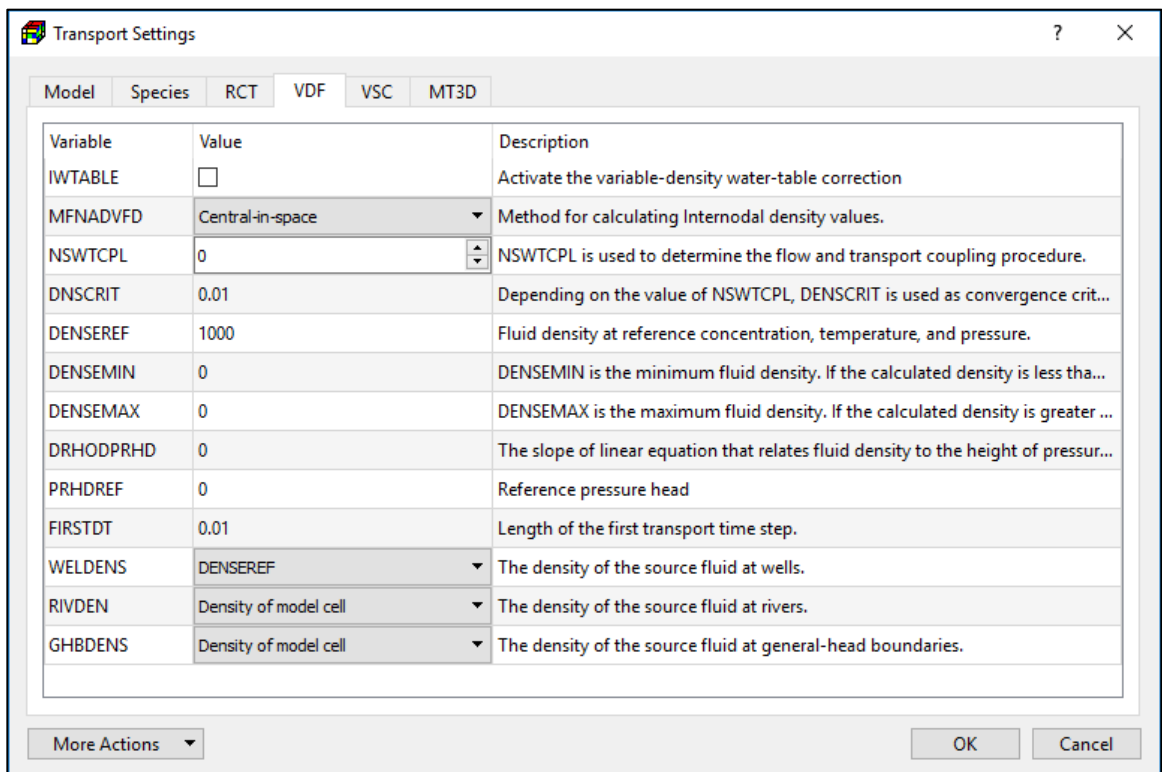
Figure 99. The VDF tab of the Transport Settings dialog box

- o If NSWTCPL > 1, NSWTCPL is the maximum number of non-linear coupling iterations for the flow and transport solutions. SEAWAT-2000 will stop execution after NSWTCPL iterations if convergence between flow and transport has not occurred.
- o If NSWTCPL = -1, the flow solution will be recalculated only for

    - The first transport step of the simulation, or
    - The last transport step of the MODFLOW time step, or
    - The maximum density change at a cell is greater than DNSCRIT.

- **DNSCRIT:** Depending on the value of NSWTCPL, DENSCRIT is used as convergence criterion or maximum density threshold.

  - o If NSWTCPL > 1, DNSCRIT is the convergence criterion for convergence between flow and transport. If the maximum fluid density difference between two consecutive implicit coupling iterations is not less than DNSCRIT, the program will continue to iterate on the flow and transport equations, or will terminate if NSWTCPL is reached.
  - o If NSWTCPL is -1, DNSCRIT is the maximum density threshold. If the fluid density change (between the present transport time step and the last flow solution) at one or more cells is greater than DNSCRIT, then SEAWAT will update the flow field (by solving the flow equation with the updated density field).

- **DENSEREF** is the fluid density at reference concentration, temperature, and pressure.

- **DENSEMIN** is the minimum fluid density. If the calculated density is less than DENSEMIN, it is set to DENSEMIN. To remove this limitation, set DENSEMIN to zero.

- **DENSEMAX** is the maximum fluid density. If the calculated density is greater than DENSEMAX, it is set to DENSEMAX. To remove the limitation, set DENSEMAX to zero.

- **DRHODPRHD** is the slope of linear equation that relates fluid density to the height of pressure head.

- **PRHDREF** is the reference pressure head.

- **FIRSTDT** is the length of the first transport time step.

- **DRNBELEV**

  - o **User-specified in the DRN Package:** the user-specified values of Elevation of Drain Bottom will be assigned to the auxiliary variable DRNBELEV in the input file to the DRN package and used for the Variable-Density Flow (VDF) process of a SEAWAT simulation.
  - o **Elevation of model cell center:** the auxiliary variable DRNBELEV will not be assigned to the input file to the DRN package, consequently the cell center elevation will be used by the VDF process of SEAWAT.

- **DRTBELEV**

  - o **User-specified in the DRT Package:** the user-specified values of Elevation of Drain Bottom will be assigned to the auxiliary variable DRTBELEV in the input file to the DRT package and used for the Variable-Density Flow (VDF) process of a SEAWAT simulation.

  - o **Elevation of model cell center:** the auxiliary variable DRTBELEV will not be assigned to the input file to the DRT package, consequently the cell center elevation will be used by the VDF process of SEAWAT.

- **GHBDENS**[42] controls the density of the source fluid at general-head boundaries.

  - o **User-specified in the GHB Package:** the user-specified values of Water Density will be assigned to the auxiliary variable GHBDENS in the input file to the GHB package and used for the Variable-Density Flow (VDF) process of a SEAWAT simulation.

  - o **Density of model cell:** the auxiliary variable GHBDENS will not be assigned to the input file to the GHB package and the calculated density of model cells will be used by the VDF process of SEAWAT by default.

- **GHBELEV:**

  - o **User-specified in the GHB Package:** the user-specified values of GHB Elevation will be assigned to the auxiliary variable GHBELEV in the input file to the GHB package and used for the Variable-Density Flow (VDF) process of a SEAWAT simulation.

  - o **Elevation of model cell center**: the auxiliary variable GHBELEV will not be assigned to the input file to the GHB package and the cell center elevation will be used by the VDF process of SEAWAT by default.

- **RIVDEN**[42] controls the density of the source fluid at rivers.

  - o **User-specified in the RIV Package:** the user-specified values of Water Density will be assigned to the auxiliary variable RIVDEN in the input file to the RIV package and used for the Variable-Density Flow (VDF) process of a SEAWAT simulation.

  - o **Density of model cell:** the auxiliary variable RIVDEN will not be assigned to the input file to the RIV package and the calculated density of model cells will be used by the VDF process of SEAWAT by default.

- **RDBTHK**

  - o **User-specified in the RIV Package:** the user-specified values of Thickness of Riverbed Sediments will be assigned to the auxiliary variable RDBTHK in the input file to the RIV package and used for the Variable-Density Flow (VDF) process of a SEAWAT simulation.

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[42] When all Density boxes in the Species tab are cleared (i.e., SEAWAT runs in the uncoupled mode), the user has the option to determine the density of the source fluid. The setting is ignored if the Density box of any of the species is checked.

- o **Difference between river bottom elevation and cell center**: the auxiliary variable RDBTHK will not be assigned to the input file to the RIV package and the difference between the river bottom elevation and cell center elevation will be used by the VDF process of SEAWAT.

- **WELDENS**[42] controls the density of the source fluid at wells.

  - o **User-specified in the WEL Package:** the user-specified values of Water Density will be assigned to the auxiliary variable WELDENS in the input file to the WEL package and used for the Variable-Density Flow (VDF) process of a SEAWAT simulation.
  - o **DENSEREF:** the auxiliary variable WELDENS will not be assigned to the input file to the WEL package and the value of DENSEREF will be used by the VDF process of SEAWAT by default.

6. **VSC Tab** (Figure 100) contains Options for the Viscosity Package of SEAWAT.
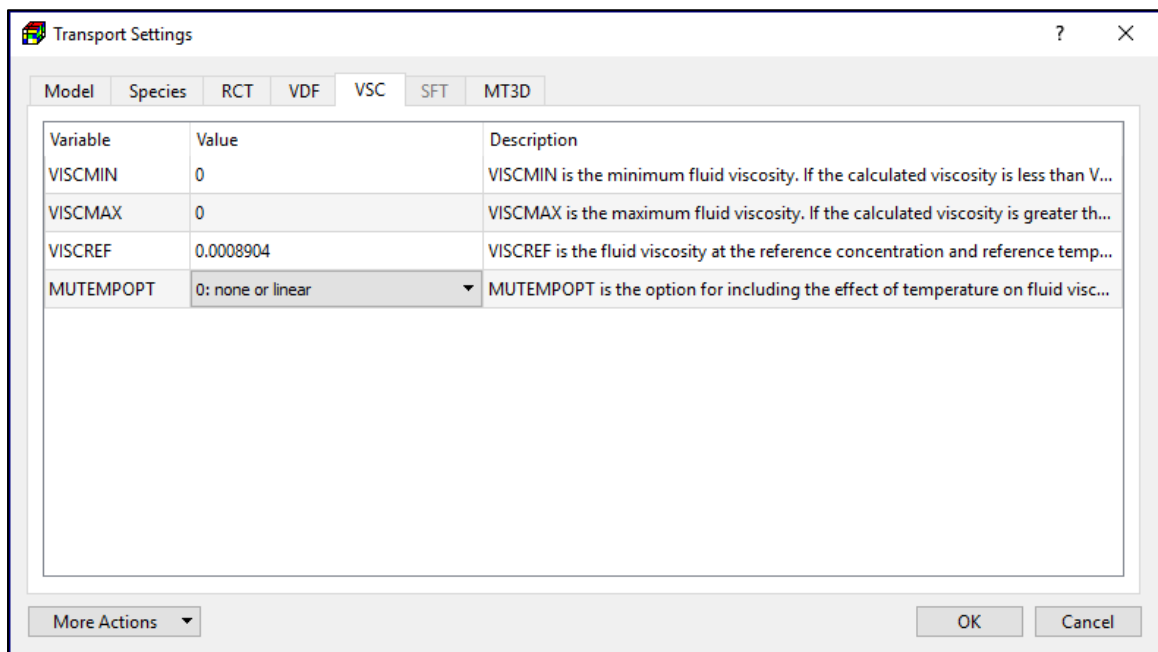
Figure 100. The VSC tab of the Transport Settings dialog box

- **VISCMIN** is the minimum fluid viscosity. If the calculated viscosity is less than VISCMIN, it is set to VISCMIN. To remove this limitation, set VISCMIN to zero.

- **VISCMAX** is the maximum fluid viscosity. If the calculated viscosity is greater than VISCMAX, it is set to VISCMAX. To remove the limitation, set VISCMAX to zero.

- **VISCREF** is the fluid viscosity at the reference concentration and reference temperature. For most simulations, VISCREF is specified as the viscosity of freshwater.

- **MUTEMPOPT** is the option for including the effect of temperature on fluid viscosity.

- o **MUTEMPOPT = 0**, the effect of temperature on fluid viscosity is defined by DMUDC and CMUREF of the species with the Viscosity box checked.
- o **MUTEMPOPT = 1**, fluid viscosity is calculated using equation 18 in (Langevin, et al., 2007). The variable MTMUTEMPSPEC and the coefficients A1 through A4 (see below) must be defined.
- o **MUTEMPOPT = 2**, fluid viscosity is calculated using equation 19 (Langevin, et al., 2007). The variable MTMUTEMPSPEC and the coefficients A1 through A5 (see below) must be defined.
- o **MUTEMPOPT = 3**, fluid viscosity is calculated using equation 20 (Langevin, et al., 2007). The variable MTMUTEMPSPEC and the coefficients A1 and A2 (see below) must be defined.

- **MTMUTEMPSPEC** is the species that corresponds to temperature. The Viscosity box of this species should NOT be checked.

- **A1** to **A5** are variables used in equations that relate dynamic viscosity to temperature. See MUTEMPOPT above for details.

7. **SFT Tab** (Figure 101) contains options for the Streamflow Transport (SFT) Package of MT3D-USGS.
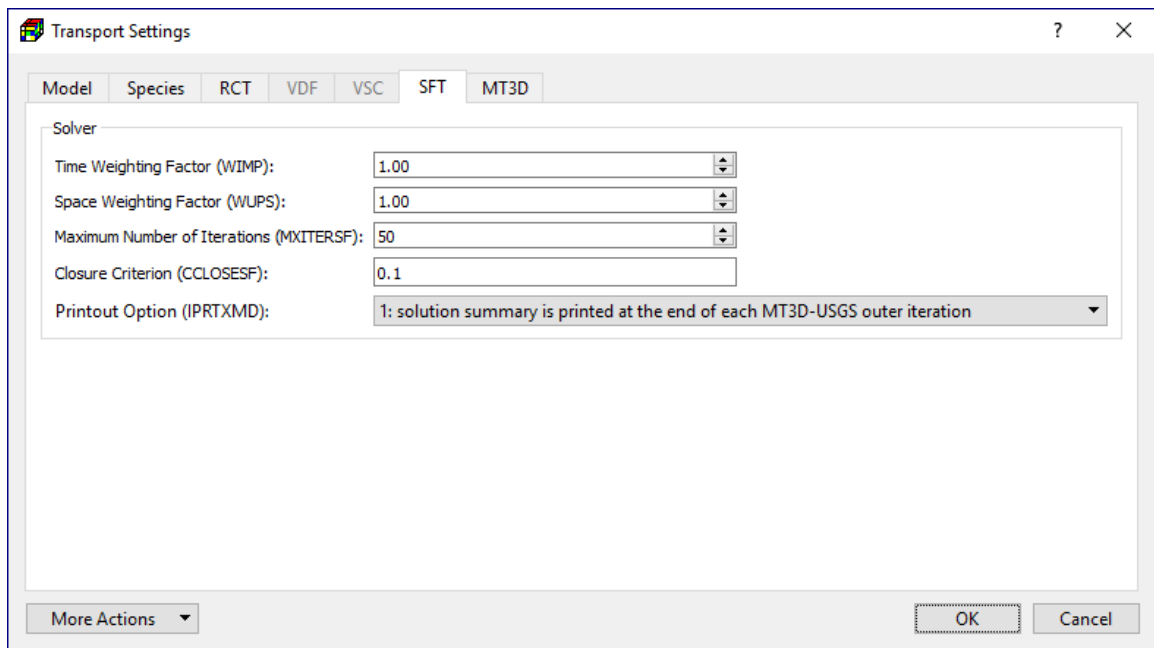
Figure 101. The SFT tab of the Transport Settings dialog box

- **Time Weighting Factor (WIMP)** is the stream solver time weighting factor. WIMP ranges between 0.0 and 1.0. Values of 0.0, 0.5, or 1.0 correspond to explicit, Crank-Nicolson, and fully implicit schemes, respectively.

- **Space Weighting Factor (WUPS)** is the space weighting factor employed in the stream network solver. WUPS ranges between 0.0 and 1.0. Values of 0.0 and 1.0 correspond to a central-in-space and upstream weighting factors, respectively.
- **Maximum Number of Iterations (MXITERSF)** is the maximum number of iterations the SFT solver can use to find a solution of the stream transport problem.
- **Closure Criterion (CCLOSESF)** is the closure criterion for the SFT solver.
- **Printout Option (IPRTXMD)** controls the printout from the SFT Solver.
8. **MT3D Tab** (Figure 102) contains options and control data of MT3D.
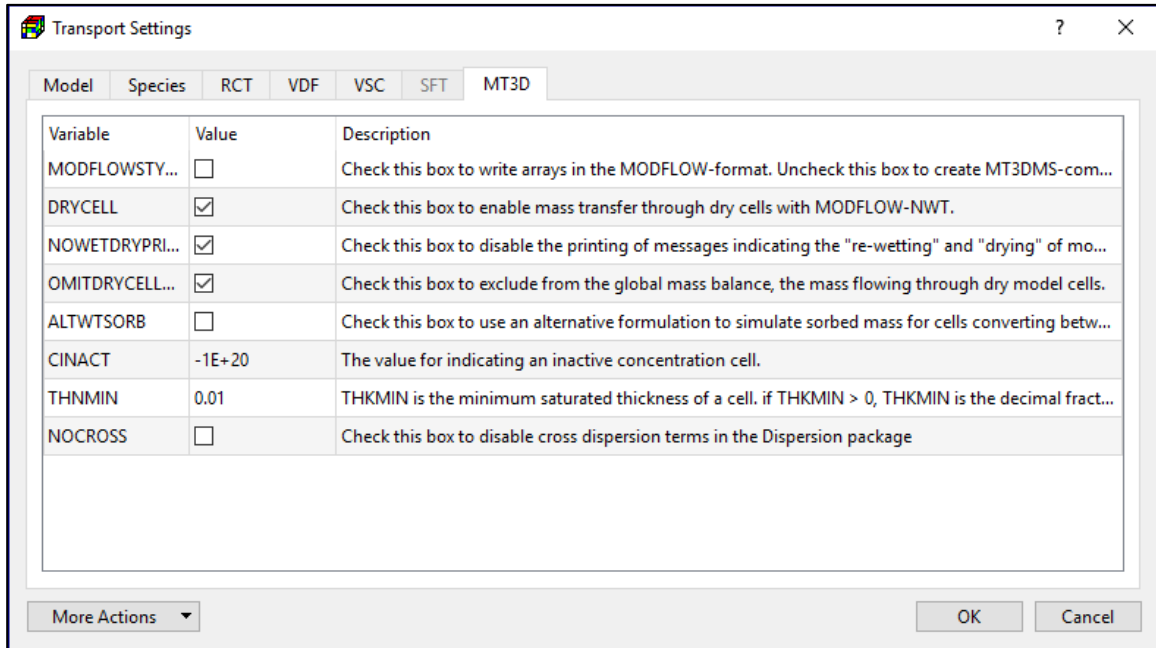
Figure 102. The MT3D tab of the Transport Settings dialog box

- **MODFLOWSTYLEARRAY**: Check this box to write arrays in the MODFLOW-format. Uncheck this box to create MT3DMS-compatible input files.

- **DRYCELL**: Check this box to enable mass transfer through dry cells with MODFLOW-NWT.

- **NOWETDRYPRINT**: Check this box to disable the printing of messages indicating the "re-wetting" and "drying" of model cells to the model run listing file.

- **OMITDRYCELLBUDGET**: Check this box to exclude from the global mass balance, the mass flowing through dry model cells.

- **ALTWTSORB**: Check this box to use an alternative formulation to simulate sorbed mass for cells converting between wet and dry.

- **CINACT** is the value for indicating an inactive concentration cell.

- **THKMIN** is the minimum saturated thickness of a cell.

  o if THKMIN > 0, THKMIN is the decimal fraction of the model layer thickness,

o   if THKMIN< 0, absolute value of THKMIN is used.

- **NOCROSS**: Check this box to disable cross dispersion terms in the Dispersion package. For most simulations, you should retain the cross-dispersion terms because they typically improve accuracy. For complex problems resulting in negative concentrations, the NOCROSS option provides a way to determine the cause of the negative concentrations.

3.8.3.2.   Initial Concentration

At the beginning of a transport simulation, MT3D and SEAWAT require the initial concentration of each active species at each active concentration cell, i.e. ICBUND > 0.

3.8.3.3.   Packages

3.8.3.3.1. Advection (ADV)

The following parameters are defined in the Advection (ADV) Package dialog box (Figure 103).
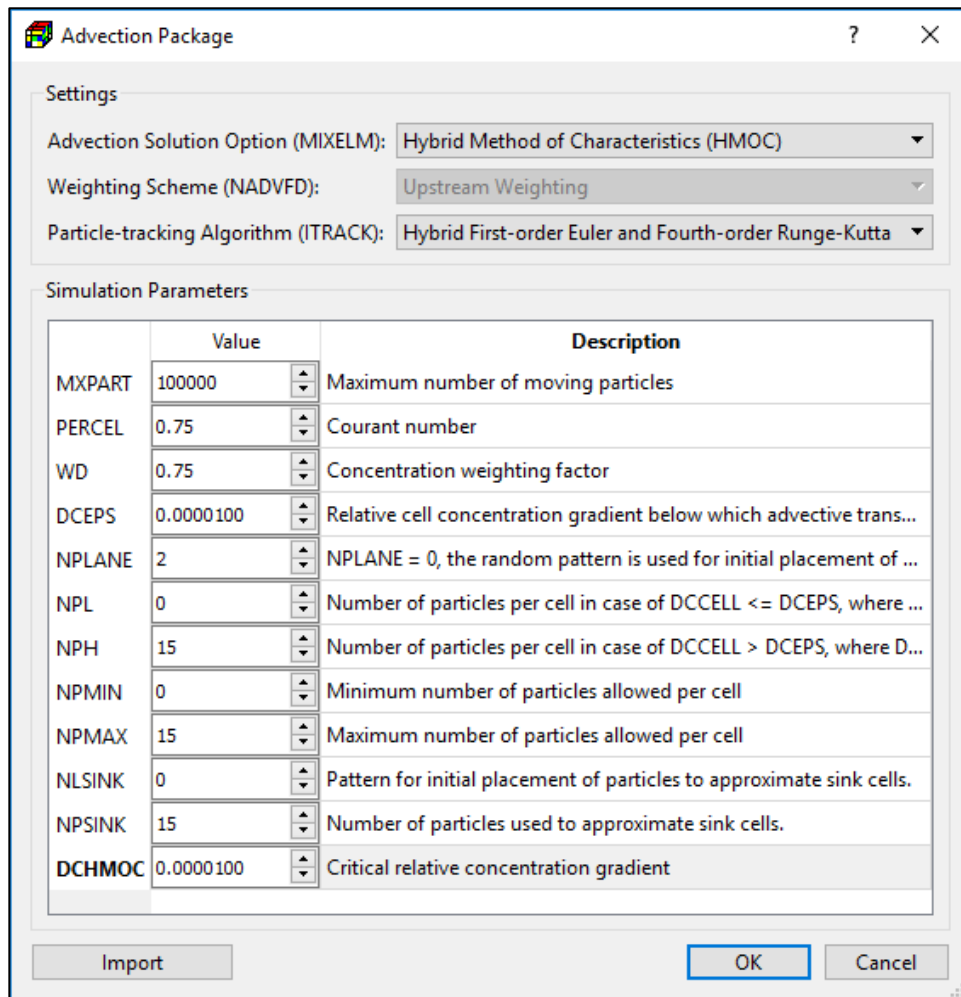
Figure 103. The Advection Package dialog box

1. **Settings**
   - **Advection Solution Option (MIXELM):**
     - o **Third-order TVD Scheme (ULTIMATE)** is based on the ULTIMATE algorithm (Leonard, 1988), which is in turn derived from the earlier QUICKEST algorithm (Leonard, 1979). With the ULTIMATE scheme, the solution is mass conservative, without excessive numerical dispersion and artificial oscillation.
     - o **Finite-Difference Method** is implicit with the Generalized Conjugate Gradient solver (GCG) package. Due to the problems of numerical dispersion and artificial oscillation, the upstream finite difference method is only suitable for solving transport problems not dominated by advection, see p. 22 in (Zheng, et al., 1999) for details. When the Peclet number P_e ($P_e = \Delta x / \alpha L$; Δx is grid spacing and αL is the longitudinal dispersivity) is smaller than two, the upstream finite difference method is reasonably accurate. However, it is advisable to use the upstream finite difference method for obtaining first approximations in the initial stages of a modeling study.
     - o **Forward Tracking Method of Characteristics (MOC)** has been widely used. One of the most desirable features of the MOC technique is that it is virtually free of numerical dispersion that poses serious difficulty in many numerical schemes. The major drawback of the MOC scheme is that it can be slow and requires a large amount of computer memory when many particles are required. Also, the computed concentrations sometimes tend to show artificial oscillations.
     - o **Backward Tracking Method of Characteristics (MMOC)** uses one particle for each finite-difference cell and is normally faster than MOC. At each new time level, a particle is placed at the nodal point of each finite-difference cell. The particle is tracked backward to find its position at the old time. The concentration associated with that position is used to approximate the advection-relevant average concentration at the cell, where the particle is placed. MMOC is free of artificial oscillations if implemented with a lower-order velocity interpolation scheme (such as linear interpolation used MT3D-USGS). However, with a lower-order velocity interpolation scheme, the MMOC technique introduces some numerical dispersion, especially for sharp front problems.
     - o **Hybrid Method of Characteristics (HMOC)** attempts to combine the strengths of the MOC and MMOC schemes by using an automatic adaptive scheme. The fundamental idea behind the scheme is automatic adaptation of the solution process to the nature of the concentration field. When sharp concentration fronts are present, the advection term is solved by MOC with moving particles dynamically distributed around each front. Away from such fronts, the advection term is solved by MMOC. The criterion for controlling the switch between the MOC and MMOC schemes is given by DCHMOC (see below).

- **Weighting Scheme (NADVFD)** is needed only when the implicit finite-difference method is used. In the finite-difference method, when computing the mass flux into a model cell by advection, the concentration values at the cell interfaces between two neighboring cells are used. For the upstream weighting scheme, the interface concentration in a direction is equal to the concentration at the upstream node along the same direction. For the central-in-space weighting scheme, the interface concentration is obtained by linear interpolation of the concentrations at the two neighboring cells. As pointed by (Zheng, et al., 1999), the central-in-space scheme does not lead to intolerable numerical dispersion when the grid spacing is regular. However, if transport is dominated by advection, the upstream weighting is preferred, as the central-in-space weighting scheme can lead to excessive artificial oscillation.

- **Particle-tracking Algorithm (ITRACK)** is used in combination with the method of characteristics.

  - **First-order Euler**: Using this algorithm, numerical errors tend to be large unless small transport steps are used. The minimum allowed transport step of all particles is determined by MT3D-USGS and is used in a transport step.

  - **Fourth-order Runge-Kutta:** The basic idea of this method is to calculate the particle velocity four times for each tracking step: one at the initial point, twice at two trial midpoints, and once at a trial end point. A weighted velocity based on values evaluated at these four points is used to move the particle to a new position. This method permits the use of larger tracking steps. However, its computational effort is considerably larger than the first-order Euler method.

  - **Hybrid First-order Euler and Fourth-order Runge-Kutta:** The option is implemented by automatic selection of the fourth-order Runge-Kutta algorithm for particles located in cells which contain or are adjacent to sinks or sources, and automatic selection of the first-order Euler algorithm for particles located elsewhere.

2. **Simulation Parameters:** Depends on the selected Solution Scheme, one or more of the following parameters may be required.

- **MXPART**: Maximum number of moving particles in a simulation.

- **PERCEL** is the number of cells (or a fraction of a cell) any particle will be allowed to move in any direction in one transport step. Generally, $0.5 \leq PERCEL \leq 1$.

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

- **DCEPS** is the relative cell concentration gradient below which advective transport is considered negligible. A value around 10^{-5} is generally adequate.

- **NPLANE:**

- o   If NPLANE = 0, the random pattern is used for initial placement of particles.
- o   If NPLANE > 0, the fixed pattern is selected for initial placement. The value of NPLANE serves as the number of "planes" on which initial particles are placed. For two-dimensional simulations in plan view, set NPLANE = 1. For cross sectional or three-dimensional simulations, NPLANE = 2 is normally adequate. Increase NPLANE if more resolution in the vertical direction is desired.

- **NPL** is the number of initial particles per cell to be placed at cells where the relative cell concentration gradient $DCCELL_{k,i,j}$ (see equation below) is less than or equal to DCEPS.

$$DCCELL_{k,i,j} = \frac{CMAX_{k,i,j} - CMIN_{k,i,j}}{CMAX - CMIN} \qquad (52)$$

  where

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

  Generally, NPL can be set to zero since advection is considered insignificant when the $DCCELL_{k,i,j}$ is less than or equal to DCEPS. Setting NPL equal to NPH causes a uniform number of particles to be placed in every cell over the entire grid.

- **NPH** is the number of initial particles per cell to be placed at cells where $DCCELL_{k,i,j}$ is greater than DCEPS. The selection of NPH depends on the nature of the flow field and the computer memory limitation. Generally, a smaller number should be used in relatively uniform flow fields and a larger number should be used in relatively nonuniform flow fields. values exceeding 16 in two-dimensional simulation or 32 in three-dimensional simulation are rarely necessary.

- **NPMIN** is the minimum number of particles allowed per cell. If the number of particles in a cell at the end of a transport step is fewer than NPMIN, new particles are inserted into that cell to maintain enough particles. NPMIN can be set to zero in relatively uniform flow fields and to a number greater than zero in diverging/converging flow fields. Generally, a value between zero and four is adequate.

- **NPMAX** is the maximum number of particles allowed per cell. If the number of particles in a cell exceeds NPMAX, all particles are removed from that cell and replaced by a new set of particles equal to NPH to maintain mass balance. Generally, NPMAX can be set to approximately two times of NPH.

- **NLSINK** is a flag indicating whether the random or fixed pattern is selected for initial placement of particles to approximate sink cells in the MMOC scheme. The convention is the same as that for NPLANE. It is generally adequate to set NLSINK equivalent to NPLANE.

- **NPMAX** is the maximum number of particles allowed per cell. If the number of particles in a cell exceeds NPMAX, all particles are removed from that cell and

replaced by a new set of particles equal to NPH to maintain mass balance. Generally, NPMAX can be set to approximately two times of NPH.

- **DCHMOC** is the critical relative concentration gradient for controlling the selective use of either MOC or MMOC in the HMOC solution scheme. The MOC solution is selected at cells where $DCCELL_{k,i,j}$ > DCHMOC. The MMOC solution is selected at cells where $DCCELL_{k,i,j} \leq DCHMOC$.

3.8.3.3.2. Dispersion (DSP)

1. **Longitudinal Dispersivity:** Select this item to define the longitudinal dispersivity of the model cells with the Data Editor. Longitudinal dispersivity is used to approximate the spreading of the solute concentration in groundwater caused by the irregular shape of the interconnected pore space and the velocity variations at the microscopic level as well as the unresolved macroscopic level. The velocity of groundwater varies according to the size of the pores and water moves faster at the internal points between soil grains than on the solid surface. This spreading is often referred to as mechanical dispersion and it occurs in all three spatial directions. Values of dispersivity used for simulations generally depend on the scale of a concentration plume being considered. While a plume "grows", it will not only undergo the microscopic mechanical dispersion but also the dispersion caused by macroscopic heterogeneities. This results in a trend of increasing dispersivity values with the scale of observation. Summaries of the scale-dependent dispersivity values can be found in (Anderson, 1984), (Gelhar, et al., 1992), and (Spitz, et al., 1996). Note that all heterogeneity, which is not explicitly represented in the model, should be incorporated into the dispersion coefficients.

2. **Diffusion Coefficient:** Select this item to define the effective molecular diffusion coefficient of the model cells with the Data Editor. describes the diffusive flux of a solute in water from an area of greater concentration toward an area where it is less concentrated. The molecular diffusion coefficient is generally very small and negligible compared to the mechanical dispersion and is only important when groundwater velocity is very low.

3.8.3.3.3. Reaction (RCT)

This menu is used for specifying the required parameters associated with the sorption and/or kinetic rate reaction types selected in Transport Settings dialog box (Figure 98). Below is a complete list of all items of this menu. The available items vary with the selected sorption and kinetic rate reaction types.

1. **Initial Concentration (Sorbed Phase):** Defines the initial Concentration for the sorbed phase.

2. **Initial Concentration (Immobile Liquid Phase):** Defines the initial Concentration for the immobile liquid phase.

3. **Distribution Coefficient**: Defines the distribution coefficient

4. **Distribution Coefficient (Mobile Domain):** Defines the distribution coefficient for the mobile domain.

5. **Distribution Coefficient (Immobile Domain):** Defines the distribution coefficient for the immobile domain

6. **Freundlich equilibrium constant:** Defines the Freundlich equilibrium constant.

7. **Freundlich equilibrium constant:** Defines the Freundlich exponent A

8. **Langmuir equilibrium constant:** Defines the Langmuir equilibrium constant

9. **Langmuir equilibrium constant:** Defines the Sorption Capacity for the Langmuir sorption

10. **Porosity (Immobile Domain):** Defines the porosity of the immobile domain.

11. **Mass Transfer Rate (Between Phases):** Defines the first-order mass transfer rate between dissolved and sorbed phases.

12. **Mass Transfer Rate (Between Domains):** Defines the first-order mass transfer rate between mobile and immobile domains.

13. **First-Order Reaction Rate (Dissolved Phase):** Defines the first-order reaction rate for the dissolved phase."));

14. **First-Order Reaction Rate (Sorbed Phase):** Defines the first-order reaction rate for the sorbed phase.

15. **Zero-Order Reaction Rate (Dissolved Phase):** Defines the zero-order reaction rate for the dissolved phase.

16. **Zero-Order Reaction Rate (Sorbed Phase):** Defines the zero-order reaction rate for the sorbed phase.

17. **Bacterium Growth Rate (Monod kinetics):** Defines the product of the total microbial concentration and maximum specific growth rate of the bacterium.

18. **Half-Saturation constant Ks (Monod kinetics):** Defines the half-saturation constant Ks for Monod kinetics.

3.8.3.3.4. Sink/Source Mixing (SSM)

This menu is used for specifying the concentration associated with the fluid of spatially distributed sources or sinks. Menu items of this menu are deactivated if the corresponding hydraulic features of *Models > MODFLOW > Packages* menu are not used (checked). The specified concentration will be used in the transport simulation if the corresponding menu item is checked. If a checked item is no longer necessary for the transport simulation, simply select the item again and deactivate it. If the concentration of a source or sink is not specified, the default value of zero is used.

Concentration values of point sources, including DRT1, GHB, FHB, MNW1, RES1, RIV, STR, and WEL, are specified using the CBC, Polyline, and Polygon input methods of the respective packages.

Evapotranspiration and Unsaturated Zone Seepage Flux are the only sinks whose concentration can be specified. The concentration of a sink cannot be greater than that of the groundwater at

the sink cell. If the sink concentration is specified greater than that of the groundwater, it is automatically set equal to the concentration of the groundwater. Therefore, setting a large sink concentration value (e.g. 1×10^{30}) to evapotranspiration ensures that the groundwater concentration is used for the computation.

The menu item Time-Variant Constant Concentration allows you to define cells with specified concentration values that vary over time. A time-variant constant concentration cell is defined by assigning a non-zero concentration value in the Data Editor. In a multiple stress period simulation, once constant-concentration condition is assigned to a cell, it remains so during the simulation, but its concentration value may vary in different stress periods. In a multispecies simulation, the constant-concentration condition applies to all species. If the constant-concentration condition does not apply to a species, assign a negative concentration value for that species.

3.8.3.3.5. Variable-Density Flow (VDF) > Prescribed Fluid Density

Use this menu item to define the fluid density for SEAWAT. This option is available only when the density effect of all species is turned off. See Species tab (Figure 97 on page 167) for details.

3.8.3.3.6. Viscosity (VSC) > Prescribed Viscosity

Use this menu item to define the fluid viscosity for SEAWAT. This option is available only when the effects of viscosity variations of all species is turned off. See Species tab (Figure 97 on page 167) for details.

3.8.3.4. GCG Solver

The GCG Solver is a general-purpose iterative solver based on the generalized conjugate gradient method for solving the system of the transport equations. A detailed description of the method can be found in (Zheng, et al., 1999). This solver must always be activated. Using this solver, dispersion, sink/source, and reaction terms are solved implicitly without any stability constraints on the transport step size. The required settings and parameters for this package are specified in the Generalized
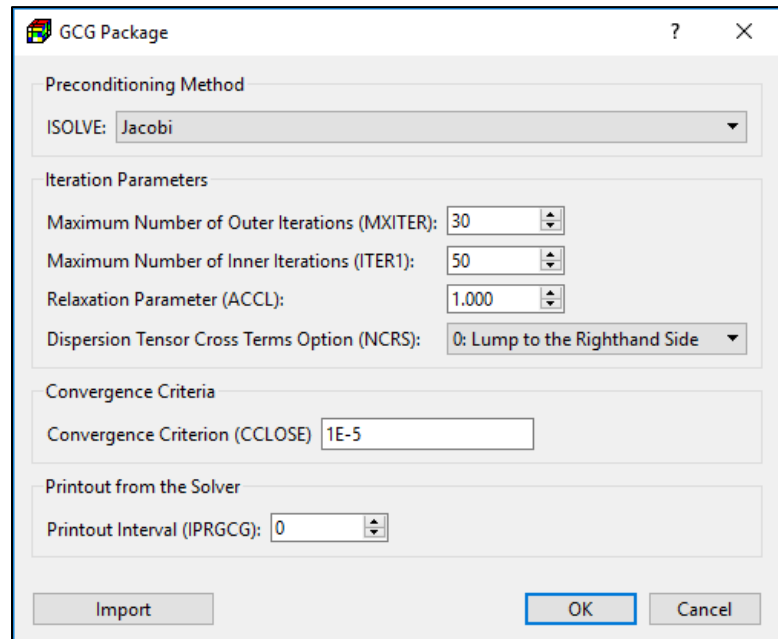
Figure 104. The GCG Package dialog box

Conjugate Gradient (GCG) dialog box (Figure 104).

1. **Preconditioning Method (ISOLVE)**: The GCG package has three preconditioning options, Jacobi, SSOR, and Modified Incomplete Cholesky. The last one usually takes less iterations than the other methods, but it requires significantly more memory.

2. **Iteration Parameters**:

   - **Maximum Number of Outer Iterations (MXITER)** and **Maximum Number of Inner Iterations (ITER1)**: The GCG solver has two iteration loops, an inner and an outer loop. Similar to the PCG solver of MODFLOW, all coefficients in the (transport-) matrix A and the right-hand-side vector b remain unchanged during inner iterations. The inner loop continues until ITER1 – iterations are executed, or the convergence criterion is met. If some of the coefficients in A are dependent on the concentration being solved, as in the case of nonlinear sorption, they must be updated in outer iterations. Therefore, MXITER should be set greater than one only when a nonlinear sorption isotherm is included in the simulation. For ITER1, a value between 30 and 50 should be adequate for most problems.

   - **Relaxation Factor (ACCL)** is only used for the SSOR option; a value of 1.0 is generally adequate.

   - **Dispersion Tensor Cross Terms Option (NCRS):** NCRS is a flag for treatment of dispersion tensor cross terms. NCRS=0, lump all dispersion cross terms to the right-hand side of the system of transport equations. It is approximate but highly efficient. NCRS=1, include full dispersion tensor. This option is memory intensive. However, for critical applications the full dispersion tensor should be included.

3. **Concentration Closure Criterion (CCLOSE)** is the convergence criterion in terms of relative concentration. A value between 10^{-6} and 10^{-4} is generally adequate. Before solving the system of transport equations, it is normalized by dividing the concentration terms by the maximum concentration of all cells. When the change of the normalized concentration at all cells during an inner iteration is less than or equal to CCLOSE, iteration stops. When it takes only one inner iteration to converge, the solution is considered to have converged and the simulation proceeds to the next transport step.

4. **Printout Interval (IPRGCG)**: The maximum concentration changes are printed out whenever the iteration number is an even multiple of this printout interval. Set it to zero for printing only at the end of each stress period.

3.8.3.5. Output Control

The available options of the Output Control (MT3D/SEAWAT) dialog box are described as follows.

1. **Output Options Tab** (Figure 105)

   - **SAVUCN** indicates whether the calculated concentration values should be saved in binary files which are used by PM for visualization. The default file names of the binary

files are MT3Dnnn.UCN for the dissolved phase and MT3Dnnns.UCN for the sorbed phases, where nnn is the species number.

Figure 105. The Output Options tab of the Output Control (MT3D/SEAWAT) dialog box

- **IFMTCN** indicates whether the calculated concentration values should be printed to the Run Listing file.

- **IFMTNP** indicates whether the number of particles in each cell should be printed to the Run Listing file.

- **IFMTRF** indicates whether the model-calculated retardation factor should be printed to the Run Listing file.

- **IFMTDP** indicates whether the model-calculated, distance weighted dispersion coefficient should be printed to the Run Listing File.

- **CHKMAS** indicates whether mass budget summary information should be printed to the mass budget file. The default file names of the mass budget summary files are MT3Dnnn.MAS, where nnn is the species number.

- **NPRMAS:** Mass budget summary information is printed every NPRMAS transport step, if CHKMAS is checked.

- **NPRS:** If NPRS < 0, simulation results are saved every NPRS transport steps (note that transport step counter starts at 0 within each flow time step.) If NPRS = 0, simulation results are saved at the end of each stress period. If NPRS > 0, simulation results are saved at the time points defined in Output Times.

2. **Output Times Tab** (Figure 106)
   - **Table**: The table contains the times at which the simulation results are saved and/or printed. Time values are expressed in the simulation time.

   - **Start Time, End Time,** and **Time Interval**: You can generate a list of output times by specifying the Start Time, End Time, and Time Interval, then clicking the Apply button. Once the list of output times is generated, you may modify the output time values on the table. Those time values will be sorted in ascending order when you close the dialog box.

- **Set Default:** Click this button to set Start Time to zero, End Time to the total simulation length of the flow simulation, Time Interval to one tenth of the total simulation length, and then populate the table accordingly.

3.8.3.6. Run

Select this menu item to open the Run MT3D dialog box (Figure 107) or Run SEAWAT dialog box
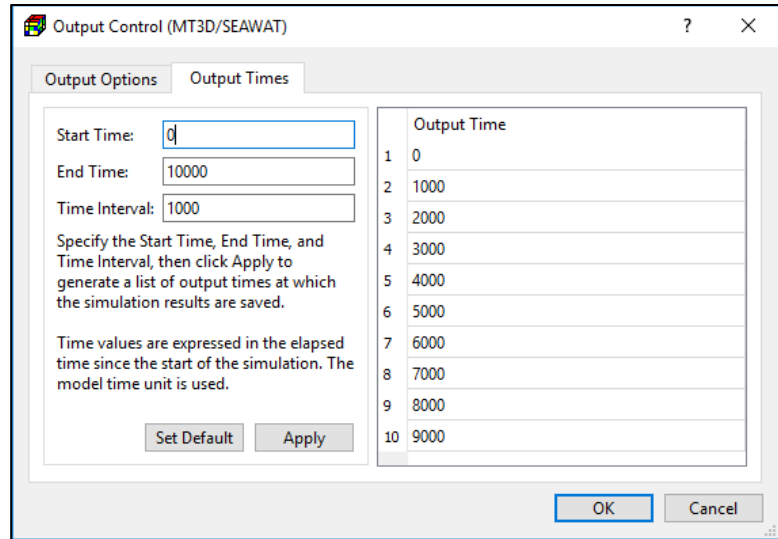
Figure 106. The Output Times tab of the Output Control (MT3D/SEAWAT) dialog box

according to the transport model selected in the Transport Settings dialog box (Section 3.8.3.1). The Run MT3D or Run SEAWAT dialog box can be used to start a transport simulation or to build input files. The available settings of the dialog box are described below.

1. **Table**

   - ⚒ **The build box.** Prior to running a transport simulation, PM uses the user-specified data to build input files for MT3D (or SEAWAT). An input file will be built if its build box is checked. If an input file does not exist or the input data has been modified since the last build, its build box will be checked automatically.

   - **Package** is the name of the package of the flow model.

   - **Filename** is the name of the input file.

   - **Status** shows the status (such as Ready, Not Exist, etc.) of the input file.
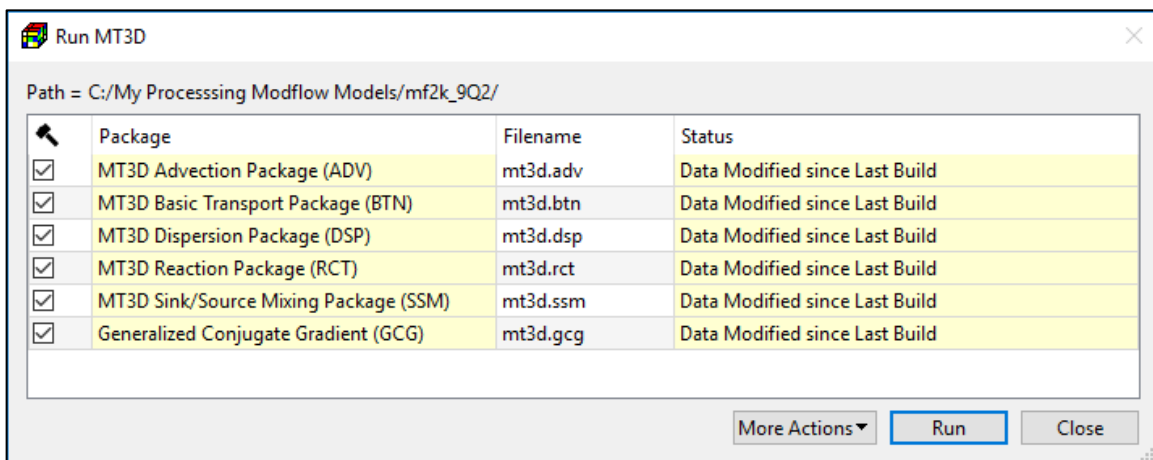
Figure 107. The Run MT3D dialog box

2. **More Actions**

   - **Inspect Model Data:** Select this to check the correctness and consistency of the model data. The inspection report will be saved in the *mt3d_inspection_log.txt* or *seawat_inspection_log.txt* file.

   - **Build Input Files:** Select this to build the input files with the checked build boxes. The name file *mt3d.nam* or *seawat.nam* will also be built. The build log is stored in the *mt3d_build_log.txt* or *seawat_build_log.txt* file.

   - **Rebuild All Input Files:** Select this to rebuild all input files, except for existing input files that are marked as read-only. The build log is stored in the *mt3d_build_log.txt* or *seawat__build_log.txt* file.

3. **Run:** Click this button to build input files with the checked build boxes and the start the transport simulation.

   - If *Constant Density Transport (MT3D-USGS)* is selected as the transport model, the simulation will be carried out by the executable file of MT3D-USGS defined in the Preferences dialog box (Figure 26). The transport process will be density-independent.

   - If *Constant Density Transport (MT3DMS)* is selected as the transport model, the simulation will be carried out by the executable file of MT3DMS defined in the Preferences dialog box (Figure 26). The transport process will be density-independent.

   - If *Variable Density Flow and Transport (SEAWAT)* is selected as the transport model, the simulation will be carried out the executable file of SEAWAT defined in the Preferences dialog box (Figure 26). The transport process can be density-dependent.

   The transport simulation progress will be displayed in the MT3D-USGS, MT3DMS or SEAWAT Output window. You may terminate the simulation at any time by clicking on the Terminate button.

3.8.3.7.   View

3.8.3.7.1. Run Listing File

Select this menu item to use the Text Editor (see Section 3.4.11) to display the run listing file mt3d.list or seawat.list.

3.8.3.7.2. Scatter Chart

Select *View > Scatter Chart* to display the scatter chart based on the concentration data of the dissolved phase. The use of the Concentration Scatter Chart dialog box is identical as the Head Scatter Chart dialog box (see Section 3.8.1.5.3), with the following exceptions:

1. **Species dropdown box** is displayed on the lower-left corner of the dialog box. Use this dropdown box to select a species of interest.
2. The simulated concentration data of the selected species is used in the Chart and the Data tab.

3.8.3.7.3. Line Chart

Select *View > Line Chart* to display the time-series chart based on the concentration data of the dissolved phase. The use of the Concentration Line Chart dialog box is identical as the Head Line Chart dialog box (see Section 3.8.1.5.4), with the following exceptions:

1. **Species dropdown box** is displayed on the lower-left corner of the dialog box. Use this dropdown box to select a species of interest.
2. The simulated concentration data of the selected species is used in the Chart and the Data tab.

3.8.3.7.4. Mass Budget Summary

Select this menu item, and then select a species to display the mass budget summary file of that species. The default file names of the mass budget summary files are MT3Dnnn.MAS, where nnn is the species number. Refer to (Neville, 2006) for details about interpreting the MT3D mass budget.

3.8.3.7.5. Concentration Summary

Select this menu item, and then select a species to create a time-history of the average concentration of the model. The calculation is based on the simulated concentration values (stored in the MT3Dnnn.ucn file, where nnn is the number of a species) and the water volume (see Section 3.8.1.5.5 for details) of the model. The calculation results are stored in a comma-separated value file consisting of a number of records. Each record includes the following terms.

- **SimulationTime** is the simulation time at which the simulated concentration values are stored in the MT3Dnnn.ucn file. Since the total amount of water in the model must be calculated as well, the average concentration will not be calculated for the SimulationTime that does not lie between the date/time of the first and last head results.

- **Period** is the stress period where SimulationTime belongs to.

- **TimeStep** is the time step within the given Period where SimulationTime belongs to.

- **Date** is the calendar date in the form of year-month-day. The date corresponds to the given simulation time.

- **Volume** [L^3] is the total amount of water in the model. This value is calculated in the same way as the **Volume** described in Section 3.8.1.5.5.

- **Mass** [L^3 x concentration unit] is the calculated as follows.

$$Mass = \sum_{i=0}^{n} (vs_i + vsy_i) \times c_i$$

  where

  n is the total number of model cells,

---

c_i is the solute concentration of the selected species in the ith cell at the given simulation time,

vs_i is the volume of water stored in the ith cell due to compressibility, and

vsy_i is the volume of water stored in the pore space of the ith cell.

The values of vs_i and vsy_i are calculated in the same way as described in Section 3.8.1.5.5. It is assumed that vs_i and vsy_i have the same concentration c_i.

- **Concentration** is calculated as Mass/Volume, and has the same unit as your input concentration values.

3.8.3.7.6. Production Concentration Summary

Select this menu item, and then select a species to create a time-history of the concentration of the extracted groundwater at the pumping wells. The calculation is based on the simulated concentration values (stored in the MT3Dnnn.ucn file, where nnn is the number of a species) and the pumping rates (stored in the modflow.flow file) at well cells. The calculation results are stored in a comma-separated value file consisting of a number of records. Each record includes the following terms.

- **SimulationTime** is the simulation time since the start of the simulation at which the simulated concentration values are stored in the MT3Dnnn.ucn file. Since the total amount of water in the model must be calculated as well, the average concentration will not be calculated for the SimulationTime that does not lie between the date/time of the first and last flow results.

- **Period** is the stress period where SimulationTime belongs to.

- **TimeStep** is the time step within the given Period where SimulationTime belongs to.

- **Date** is the calendar date in the form of year-month-day. The date corresponds to the given simulation time.

- **Well** is the well name. The cells with the same well name will be considered a part of the well. If the well name of a well cell is not specified, the default name "row_column" will be used, where row/column are the model row and column of the well cell. Consequently, the cells in various layers of that row/column location will be considered a part of that well.

- **PumpingRate** [L^3/T] is the sum of the pumping rates of the model cells that belong to the given well.

- **MassRate** [L^3/T x concentration unit] is the sum of [pumping rate x concentration] of the model cells that belong to the given well.

- **Concentration** is the concentration of the water extracted by the well. The value is calculated as [Concentration = MassRate / PumpingRate] and has the same unit as your input concentration values.

3.8.4. PEST

This menu provides the interface to PEST (Doherty, 2016) and/or BeoPEST (Hunt, et al., 2010).

Table 4 shows a list of estimable parameters through PEST or BeoPEST within PM. The estimable aquifer parameters depend on the selection of the internal flow package and layer types[43]. During a parameter estimation process, PEST searches optimum parameter values for which the sum of squared deviations between model-calculated and observed values at the observation points is reduced to a minimum.

Table 4. Estimable Parameters through PEST/BeoPEST within PM

Packages	Parameters
Block-Centered Flow (BCF)	Confined: T, S, and VCONT[44] Unconfined: HK, Sy, and VCONT[44] Limited Convertible: T, S, Sy, and VCONT[44] Full Convertible: HK, S, Sy, and VCONT[44]
Layer-Property Flow (LPF)	All layer types: HK, HANI, VANI, VK, Ss, and Sy.
Upstream-Weighting (UPW)	All layer types: HK, HANI, VANI, VK, Ss, and Sy.
Drain (DRN)	Drain conductance
Drain with Return Flow (DRT)	Drain conductance
Evapotranspiration (EVT)	Maximum ET Flux
Evapotranspiration Segments (ETS)	Maximum ET Flux
General-Head Boundary (GHB)	Boundary conductance
Horizontal-Flow Barrier (HBF)	Hydraulic characteristic
Interbed Storage (IBS)	Inelastic Storage Factor
Recharge (RCH)	Recharge flux
River (RIV)	Riverbed conductance
Reservoir (RES1)	Vertical hydraulic conductivity of reservoir bed
Stream (STR)	Streambed conductance
Streamflow-Routing (SFR2)	Hydraulic conductivity of the streambed
Unsaturated-Zone Flow (UZF1)	Infiltration rate
Well (WEL)	Flow rate

Follow the steps below to define observations and estimable parameters that are required by PEST and BeoPEST:

1. **To define observation points and observation values**
   - See Section 3.5.3 for details.

2. **To define an estimable parameter**

---

[43] When BCF is selected as the internal flow package, the estimable aquifer parameters depend on the layer type (as listed in Table 3) regardless of the Calculated/User-specified settings in the Layer Property dialog box.
[44] VCONT is used only if the layer is not the bottom layer.

- Select a parameter from the Parameters menu or select a package from *Models > MODFLOW > Packages* menu
- Assign an initial guess of the parameter value and a parameter number to cells within an area where the parameter value should be estimated.
  - o The initial guess of the parameter value must be non-zero.
  - o The parameter number must be unique within a parameter type (e.g., T, S or Ss) and may be any integer ranging between 0 and 10000. Set the parameter number to zero, if the specified parameter value should not be estimated.
- Select *Model > PEST > Settings* to open the PEST Settings dialog box. If this dialog box is opened the first time, the defined parameters will be listed in the Parameters Tab. Otherwise, select *More Actions > Search for Parameters* to find the new parameters.

3.8.4.1. Settings

The required inputs and options for running PEST and/or BeoPEST are specified in the PEST Settings dialog box (Figure 108). The variable names used in this dialog box are identical as those given in the PEST Manual (Doherty, 2016). Briefly explanations of these variables are provided below. Consult the PEST Manual for details.

1. **Operation Mode**
   - **Parameter Estimation:** PEST will run in the "estimation" mode and will use the available information to estimate parameters defined in the Parameters Tab by running the model as many times as needed. Solution of the inverse problem can be

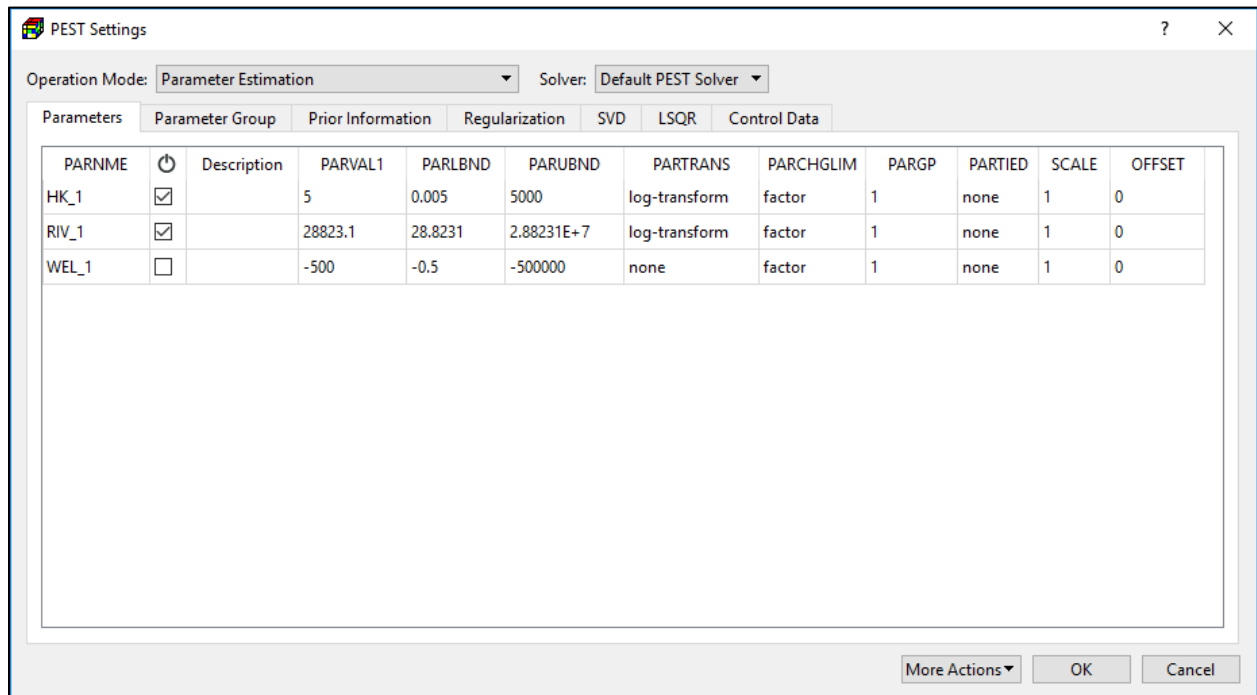| PARNME	⏻	Description	PARVAL1	PARLBND	PARUBND	PARTRANS	PARCHGLIM	PARGP	PARTIED	SCALE	OFFSET
HK_1	☑		5	0.005	5000	log-transform	factor	1	none	1	0
RIV_1	☑		28823.1	28.8231	2.88231E+7	log-transform	factor	1	none	1	0
WEL_1	☐		-500	-0.5	-500000	none	factor	1	none	1	0

Figure 108. The Parameters tab of the PEST Settings dialog box

based on the Gauss-Marquardt-Levenberg method. Alternatively, singular value decomposition or LSQR can be used to solve the inverse problem. When many parameters require estimation, LSQR is much faster than that of singular value decomposition.

- **Sensitivity Analysis:** When this option is selected, the maximum number of optimization iterations (see NOPTMAX in the Control Data tab) will be set to -1. PEST will run in the "estimation" mode but will terminate execution immediately after it has calculated the Jacobian matrix for the first time. The parameter covariance, correlation coefficient and eigenvector matrices will be written to the run record file, and parameter sensitivities will be written to the sensitivity file; these are based on the initial parameter set defined in the Parameters tab.

- **Run Model with the Specified PARVAL1 Values:** When this option is selected, the maximum number of optimization iterations (see NOPTMAX in the Control Data tab) will be set to 0. PEST will run in the "estimation" mode but will not calculate the Jacobian matrix. Instead it will terminate execution after just one model run. This setting can thus be used when you wish to calculate the objective function corresponding to a parameter set and/or to inspect observation residuals corresponding to that parameter set.

- **Regularization**: To run PEST in the regularization mode, you must supply at least one prior information equation with the name of the observation group (OBGNME) starting with "regul". As described in (Doherty, 2016), *when run in "regularization" mode, PEST employs two objective functions rather than one. One of these is called the "measurement objective function" while the other is referred to as the "regularization objective function". The lower is the former, the better do model-calculated quantities match their field-measured counterparts. The lower is the latter, the better do parameter values respect mathematical expressions of expert knowledge encapsulated in observations or prior information equations that are dedicated to this purpose.* Refer to the PEST book (Doherty, 2015) and Chapter 9 of the Part I of the PEST Manual (Doherty, 2016) for details about the regularization mode.

2. **Solver:** The selected solver is used to solve the linearized inverse problem during each iteration of the overall inverse process. As discussed in (Doherty, 2015), the Singular value decomposition (SVD) and the LSQR algorithm introduce numerical stability to solution of an ill-posed inverse problem. In most cases, *SVD Mode1, SVD Mode 2, or LSQR* should be used instead of the PEST's default solver. *SVD Mode 2* is superior than *SVD Mode 1* for cases involving many observations as the formation of the matrix for the inverse problem may take a considerable amount of time under these circumstances. A benefit of LSQR over SVD is its speed. If parameters number more than a couple of thousand, SVD can become very slow. This is not the case for LSQR which can happily handle tens of thousands of parameters and hundreds of thousands of observations.

3. **More Actions:** This menu acts on the Parameter Table (see below), the functions of the menu items are as follows.

- **Update**: Update PARVAL1 of the Parameter Table with the estimated parameter values.

- **Delete**: Delete the selected row from the Parameter Table.

- **Clean Up**: Delete unused parameters from the Parameter Tab. An estimable parameter becomes unused when its parameter number no longer exists in all cells of the respective parameter type.

- **Search for Parameters**: Search for estimable parameters and add them to the Parameter Tab.

4. **Parameters Tab** contains a Parameter Table that lists the estimable parameters and their properties.

- **PARNAM** is the parameter name and is a combination of that parameter number and the short name of the aquifer parameter (i.e., HK, HANI, VK, VANI, SS, SY, T, S or VCONT) or package. For example, if parameter numbers 1 and 2 are specified for the Recharge Package, the parameter names are RCH_1 and RCH_2. Similarly, if parameter numbers 3 is assigned to HK, the parameter name is HK_3. Modification of the parameter names is not allowed. Note that when switching between internal flow packages (i.e., BCF, LPF, and UPW), some aquifer parameters might become inestimable. For example, PEST cannot estimate values of T and S when using the LPF Package, because the input file of the LPF Package does not include T and S values.

- ⏻: Check/uncheck the boxes in this column to activate/deactivate parameters. The value of a parameter will only be estimated if its box checked. Otherwise the user-specified cell values will be used for the simulation.

- **Description** contains optional text string to describe the parameter.

- **PARVAL1** is the initial value of the parameter. The default value is the arithmetical mean of the cell values of that parameter.

- **PARLBND and PARUBND:** The parameter's lower bound (PARLBND) and upper bound (PARUBND) default to two orders of magnitude lower and higher than PARVAL1, respectively. For adjustable parameters, PARVAL1 must lie between these two bounds. For fixed and tied parameters, PARLBND and PARUBND are ignored.

- **PARTRANS** controls the parameter transformation.

  o **None**: No transformation takes place.
  o **Log-transformed** ensures that the estimated value is always positive and is recommended for transmissivities and hydraulic conductivities. A parameter, which can become zero or negative during the parameter estimation process, must not be log-transformed; hence if a parameter's lower bound is zero or less, PEST will disallow logarithmic transformation for that parameter.
  o **Fixed**: The parameter is fixed at PARVAL1 and takes no part in the optimization process.

- o **Tied**: The parameter is linked to another parameter. A tied parameter plays only a limited role in the estimation process. The *parent* parameter, to which the tied parameter is linked, takes an active part in the parameter estimation process and must be neither fixed nor tied itself. During the parameter estimation process, the value of the tied parameter maintains the same ratio to the parent parameter as the ratio of their initial values.

- **PARCHGLIM** is used to designate whether the value change of an estimable parameter is relative-limited or factor-limited. See the discussion on RELPARMAX and FACPARMAX in the Control Data Tab below. PARCHGLIM is not used for a fixed parameter.

- **PARGP** is the number of the parameter group to which a parameter belongs. Parameter groups are discussed below.

- **PARTIED** is the parent parameter to which is parameter is linked.

- **SCALE** and **OFFSET:** Just before a parameter value is written to an input file of MODFLOW, it is multiplied by SCALE, after which OFFSET is added. The use of these two variables allows you to redefine the domain of a parameter. Because they operate on the parameter value "at the last moment" before it is sent, they take no part in the estimation process. Using SCALE and OFFSET, the parameter b_p optimized by PEST is

$$b_p = (b_m - OFFSET)/SCALE \qquad (53)$$

where b_m is the parameter seen by the model. If you wish to leave a parameter unaffected by SCALE and OFFSET, enter the SCALE as 1.0 and the OFFSET as 0.0.

5. **Parameter Group Tab** (Figure 109)**:** In PEST, the input variables that define how derivatives are calculated pertain to parameter groups rather than to individual parameters. Thus, derivative data do not need to be entered individually for each parameter; however, if you wish, you can define a group for every parameter and set the derivative variables for each parameter separately.

- **Description** is an optional description of the parameter group.

- **INCTYP and DERINC:** INCTYP is the method by which parameter increments are calculated. DERINC is the absolute or relative parameter increment. The option for INCTYP are as follows:

  - o **Relative**: The parameter increment is calculated as a fraction of the current value of that parameter; that fraction is specified in DERINC. A DERINC value of 0.01 is often appropriate.
  - o **Absolute**: The parameter increment is fixed at the value of DERINC. No suggestion for an appropriate DERINC value can be provided for this option; the most appropriate increment will depend on the parameter magnitudes.
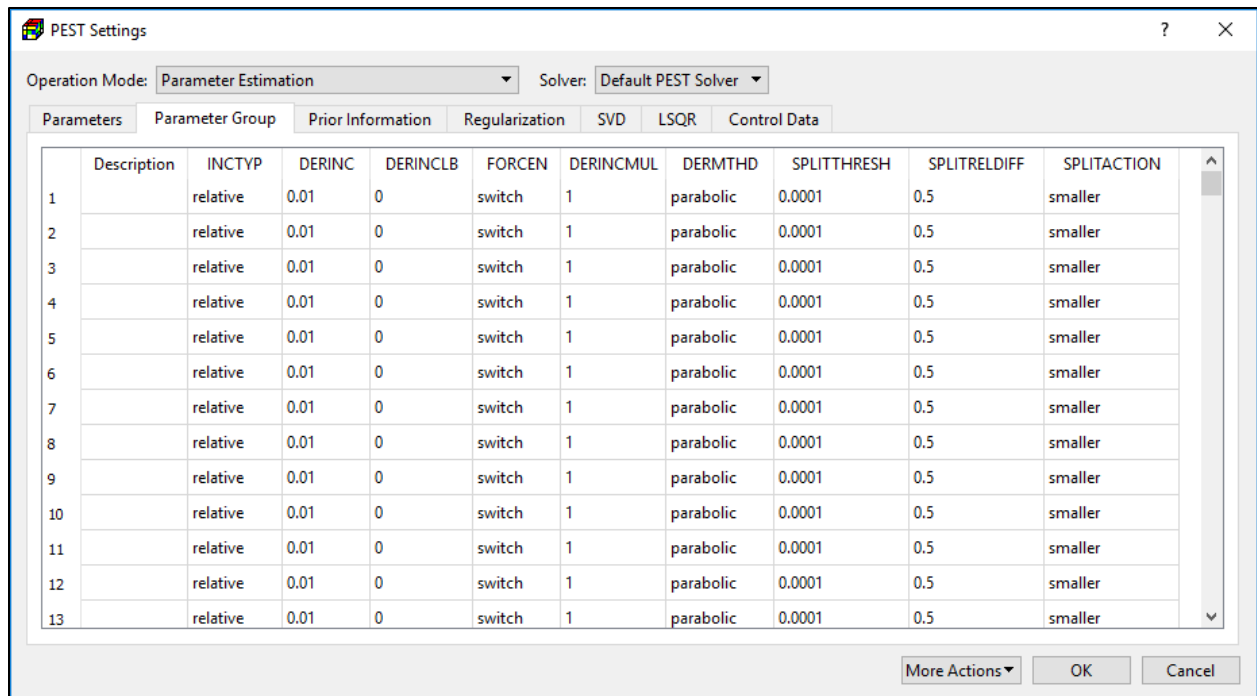
Figure 109. The Parameter Group tab of the PEST Settings dialog box

- o **Rel_to_max**: The parameter increment is calculated as a fraction of the group member with highest absolute value, that fraction again being DERINC. A DERINC value of 0.01 is often appropriate. If a group contains members, which are fixed and/or tied, the values of these parameters are used when calculating parameter increments.

- **DERINCLB** is the lower bound of relative parameter increment; ignored if INCTYP is *Absolute*. If a parameter increment is calculated as *Relative*, it may become too low if the parameter values become very small. And, if a parameter increment is calculated as *Rel_to_max*, it may become too low if the modulus of the largest parameter in the group is very small. A parameter increment becomes "too low" if it does not allow reliable derivatives to be calculated with respect to that parameter because of round off errors incurred in the subtraction of nearly equal model generated values. DERINCLB is used to bypass this possibility. Set DERINCLB to zero if you do not wish to place a lower limit on parameter increments in this fashion.

- **FORCEN** determines whether higher order derivatives calculation is undertaken.

- o **Always_2**: Derivatives will be calculated using the forward difference method.
- o **Always_3**: PEST will use the central (i.e. three-point) method to calculate the derivatives. In this case, twice as many model runs as there are parameters within the group will be required. However, the derivatives will be calculated with greater accuracy and this will probably have a beneficial effect on the performance of PEST.
- o **Always_5:** PEST will use a five-point method to calculate the derivatives.

- o **Switch**: Derivatives calculations will begin using the forward difference method, switching to the central (i.e. three-point) method for the remainder of the estimation process after the relative objective function reduction between successive iterations is less than PHIREDSWH as defined in the Control Data Tab below.
- o **Switch_5:** The switch is made from forward differences to five-point derivatives under the same conditions as described in Switch above.

- **DERINCMUL** is the parameter increment multiplier; this is the value by which DERINC is multiplied when it is used to evaluate increments for any of the three central derivatives methods. Sometimes it is useful to employ larger increments for central derivatives calculation than for forward derivatives calculation. However, if the increment is raised too high, derivative precision must ultimately fall. Note that through DERINCMUL you can also reduce the increment used for central derivatives calculation if you wish. DERINCMUL plays a similar role in implementation of five-point derivatives as that which it plays in implementation of central derivatives.

- **DERMTHD** defines the method of higher order derivatives calculation.

  - o If *FORCEN* is set to *always_3* or *switch*, DERMTHD must be set to one of *outside_pts*, *parabolic* or *best_fit*; this determines the method of central derivatives calculation to be used by PEST.
  - o If *FORCEN* is set to *aways_5* or *switch_5*, DERMTHD must be either *minvar* to activate the minimum error variance alternative of the five-point methodology or to *maxprec* to activate the maximum precision alternative. Refer to Part I of the PEST Manual (Doherty, 2016) for details about these methods.

- **SPLITTHRESH, SPLITRELDIFF, and SPLITACTION:** These variables are used by "split slope analysis". See Section 3.5.7 of the Part I of the PEST Manual (Doherty, 2016) for details.

6. **Prior Information Tab** (Figure 110)**:** It often happens that we have some information concerning the parameters that we wish to optimize, and that we obtained this information independently of the current experiment. This information may be in the form of other unrelated estimates of some or all of the parameters, or of relationships between parameters. It is often useful to include this information in the parameter estimation process because it may lend stability to the process.

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

$$PILBL\ PIFAC * PARNME\ +\ PIFAC * log(PARNME)\ldots =\ PIVAL\ WEIGHT\ OBGNME \qquad (54)$$
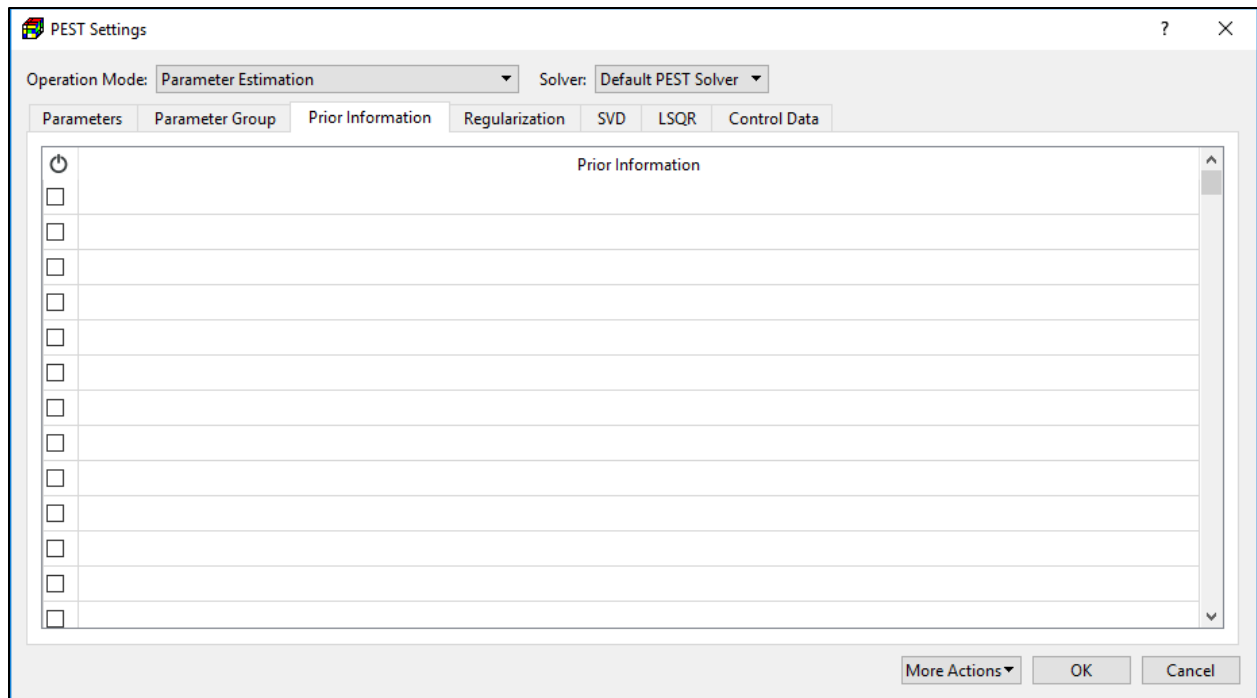
Figure 110. The Prior Information tab of the PEST Settings dialog box

The variables of the prior information equations are defined as follows. All variables and symbols must be separated from by at least one space.

- ***PILBL*** : Each prior information article must begin with a case insensitive prior information label. The label must be no more than twenty characters in length and must be unique to each prior information article.

- ***PIFAC*** and ***PARNME*** : $PIFAC$ is a parameter factor. $PARNME$ is the parameter name. Both are required. To the left of the "=" sign there are one or more combinations $PIFAC$ and $PARNME$, with a "log" prefix to $PARNME$ if appropriate. $PIFAC$ and $PARNME$ are separated by a "*" character signifying multiplication. All parameters referenced in a prior information equation must be estimable parameters; i.e., you must not include any fixed or tied parameters. Furthermore, any parameter can be referenced only once in any one prior information equation; however, it can be referenced in more than one equation.

- ***PIVAL*** is the value of the right-hand side of the prior information equation.

- ***WEIGHT***: The prior information weight should ideally be inversely proportional to the standard deviation of $PIVAL$; it can be zero if you wish but must not be negative. In practice the weights should be chosen such that the prior information equation neither dominates the objective function or is dwarfed by other components of the objective function. In choosing observation and prior information weights, remember that the weight is multiplied by its respective residual and then squared before being assimilated into the objective function.

- **OBGNME** is observation group to which the prior information belongs. *OBGNME* must be twelve characters or less in length. <u>When running PEST in the Regularization mode, *OBGNME* of at least one of the prior information equations must start with "regul"</u>. PEST can accommodate multiple regularization groups. Any observation group name starting with "regul" is a regularization group.

Some examples of prior information equations are given below, refer to the Part I of the PEST Manual (Doherty, 2016) for more details.

Example 1:

```
pi1 1.0 * par1 = 2.305 1.0 prgp
```

This prior information equation is given the label $pi1$ and has a single untransformed parameter named $par1$. This parameter has a preferred value of 2.305. This information will be included in the optimization process with a weight of 1.0 and is assigned to the observation group $prgp$.

Example 2:

```
pi1 1.0 * log(par1) = 0.362671 1.0 prgp
```

This prior information equation is similar to the previous example, with the exception that $par1$ is log-transformed. The preferred value of the log-transformed parameter is 0.362671 (= log(2.305)). Note that logs are taken to base 10.

Example 3:

```
pi2 1.0 * par + 3.4 * par3 – 2.3 * par4 = 1.09e3 3.0 prgp
```

This example shows that the left side of a prior information equation can be comprised of the sum and/or difference of a number of factor-parameter pairs; these pairs must be separated from each other by a "+" or "-" sign, with a space to either side of the sign.

Example 4:

```
pi3 1.0 * log(par1) – 1.0 * log(par2) = 1.60206 2.0 prgp
```

Prior information equations which include log-transformed parameters must express a relationship between the logs of those parameters. This equation defines the ratio between the estimated values of parameters "par1" and "par2" to be about 40.0, i.e., log(par1/par2) = log(40) = 1.60206.

7. **Regularization Tab** (Figure 111)**:** Tikhonov regularization is the most commonly used method of regularization and is incorporated in PEST. In its broadest sense, regularization is a term used to describe the process whereby many parameters can be simultaneously estimated without incurring the numerical instability that normally accompanies parameter nonuniqueness. Numerical stability is normally achieved through the provision of supplementary information to the parameter estimation process. Such supplementary information often takes the form of preferred values for parameters, or for relationships between parameters (i.e., prior information). Thus if, for a parameter, the information content of the observation dataset is such that a unique value cannot be estimated for
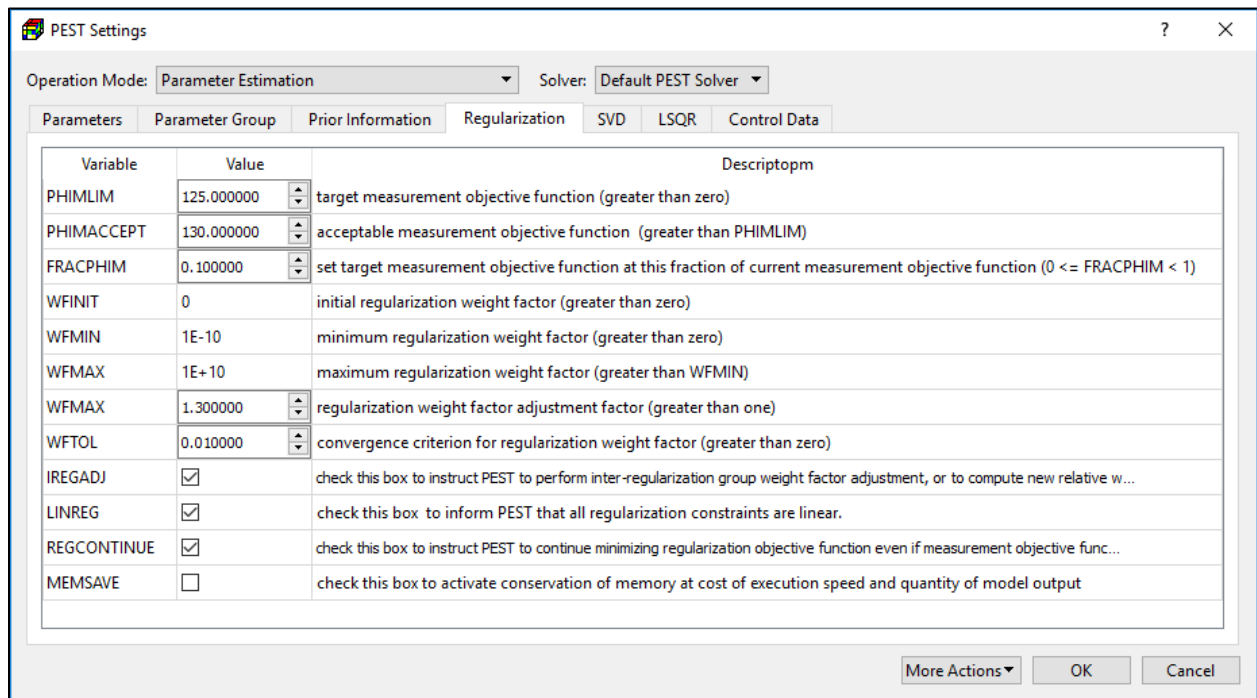
Figure 111. The Regularization tab of the PEST Settings dialog box

that parameter based on that dataset alone, uniqueness can nevertheless be achieved by using the supplementary information provided for that parameter through the regularization process. Regularization is particularly useful in estimating values for parameters which describe the spatial distribution of some property over a two- or three-dimensional model domain of a ground water model. You are no longer required to subdivide the model domain into a small number of zones of piecewise parameter constancy. Rather, a large number of parameters can be used to describe the distribution of the spatial property and PEST's regularization functionality can be used to estimate values for these parameters.

To run PEST in the regularization mode, select Regularization from the Operation Mode dropdown box, define at least one prior information equation (see above) and set the observation group (OBGNME) of the prior information equation to start with "regul", then assign appropriate values to the following parameters in the Regularization Tab.

- **PHIMLIM** is the target measurement objective function and must be greater than zero. PHIMLIM is the upper limit of the measurement objective function (i.e., the upper level of model-to-measurement misfit) that is tolerable when trying to minimize the regularization objective function. In some cases, a PEST regularization run will postdate a normal parameter estimation run. If the latter run was successful, it will have informed the user of how low the measurement objective function can be if all parameters are adjusted without reference to any regularization conditions. PHIMLIM should be set somewhat above this, for the imposition of regularization constraints will mostly result in a slight diminution of PEST's ability to fit the field data exactly.

- **PHIMACCEPT** is the acceptable measurement objective function and must be greater than PHIMLIM. During each optimization iteration, just after it has linearized the problem through calculating the Jacobian matrix, and just before it begins calculation of the parameter upgrade vector, PEST calculates the optimal value of the regularization weight factor for that iteration. This is the value which, under the linearity assumption encapsulated in the Jacobian matrix, results in a parameter upgrade vector for which the measurement component of the objective function is equal to PHIMLIM. However, due to the approximate nature of the linearity assumption, PEST may not be able to lower the measurement component of the objective function to PHIMLIM on that iteration although it uses several different values for the Marquardt lambda in attempting to do so. If it cannot lower the measurement objective function to an acceptable level, it simply accepts the upgraded parameters, proceeds to the next optimization iteration. However, if it does succeed in lowering the measurement objective function to an acceptable level, or if it has succeeded in doing this on previous iterations, then PEST slightly alters its philosophy of choosing new Marquardt lambdas, in that it now attempts to lower the regularization component of the objective function while maintaining the measurement component of the objective function below this acceptable level. This acceptable level is PHIMACCEPT; it should be set slightly higher than PHIMLIM so that PEST has some room to move.

- **FRACPHIM** set target measurement objective function at this fraction of current measurement objective function (0 ≤ FRACPHIM < 1).

- **WFINIT** is the initial regularization weight factor and must be greater than zero. During every optimization iteration PEST calculates a suitable regularization weight factor using an iterative, numerical solution procedure; its initial value for the first optimization iteration is WFINIT.

- **WFMIN** and **WFMAX** are respectively the minimum and maximum regularization weight factors and must be greater than zero. If a regularization scheme is poor, (and does not lend too much stability to an already unstable parameter estimation process), selection of appropriate values for WFMIN and WFMAX may be quite important, for these can prevent PEST from calculating outrageous values for the regularization weight factor to compensate for inadequacies of the regularization scheme.

- **WFFAC** and **WFTOL.** WFFAC is the regularization weight factor adjustment factor and must be greater than one. WFTOL is the convergence criterion for regularization weight factor and must be greater than zero. When PEST calculates the appropriate regularization weight factor to use during an optimization iteration, it uses an iterative procedure which begins at the value of the regularization weight factor calculated for the previous optimization iteration; for the first iteration, it uses WFINIT to start the procedure. In the process of finding the weight factor, PEST first travels along a path of progressively increasing or decreasing weight factor by either multiplying or

dividing the weight factor by WFFAC; it continues to do this until it has found two successive weight factors which lie on either side of the optimal weight factor for that optimization iteration. Once it has done this, it uses Newtons method to calculate the optimal weight factor, through a series of successive approximations. When two subsequent weight factors calculated in this way differ from each other by no more than a relative amount of WFTOL, the optimal weight factor is deemed to have been calculated.

- **IREGADJ:** Check this box to instruct PEST to perform inter-regularization group weight factor adjustment, or to compute new relative weights for regularization observations and prior information equations

- **LINREG**: Check this box to inform PEST that all regularization constraints are linear. As discussed in the PEST Manual, regularization constraints can be supplied through observations, through prior information, or both. Prior information relationships are always linear. Regularization constraints supplied as observations (for which the current value of pertinent relationships is calculated by the model), can be linear or nonlinear; in either case, derivatives of these relationships with respect to adjustable parameters are re-evaluated by PEST during each optimization iteration. If regularization information is entirely linear, many matrix operations carried out as part of PEST's regularization functionality do not need to be repeated from iteration to iteration. If repetition of these calculations can be avoided in parameter estimation contexts involving many regularization constraints, significant gains in efficiency can be made.

- **REGCONTINUE**: Check this box to instruct PEST to continue minimizing regularization objective function even if measurement objective function less than PHIMLIM. Under normal circumstances, when working in regularization mode, PEST ceases execution immediately if the measurement objective function falls below PHIMLIM. There are some circumstances, however, where minimization of the regularization objective function is just as important as allowing the measurement objective function to reach PHIMLIM. If this box is checked, PEST will continue optimizing regularization objective function after reached PHIMLIM.

- **MEMSAVE**: Check this box to activate conservation of memory at cost of execution speed and quantity of model output. If this box is checked, nonessential PEST tasks which are curtailed include the following:

  o The parameter covariance matrix, and matrices derived from it, are not calculated by PEST at regular intervals during the parameter estimation process for recording in the matrix file, pest.mtt; nor are these matrices calculated at the end of the inversion process for recording in the run record file pest.rec. Because the covariance matrix is unavailable, parameter uncertainties cannot be calculated, and hence are also not recorded in the run record file. (In a regularization context, these have little meaning anyway.)

o Some avenues for increasing the efficiency of regularization calculations are no longer available under the leaner storage regime that prevails when memory conservation is active (including the benefits gained through the LINREG variable and through the placing of regularization observations behind other observations involved in the parameter estimation process). This can lead to significant run-time penalties in problems involving many parameters; unfortunately, these are the very contexts in which memory conservation is most likely to be warranted.

8. **SVD Tab** (Figure 112)**:** The variables of this tab are used only if the Solver is either *SVD Mode 1* or *SVD Mode 2.*

- **MAXSING** is the number of singular values at which truncation occurs and must be greater than zero. Ideally this should be equal to the optimal dimensionality of the solution space. This is difficult to determine though the SUPCALC utility described in part II of the PEST Manual (Doherty, 2016) may provide some help in this regard. Normally the role of singular value decomposition is to achieve numerical stability of the inversion process rather than to provide regularization. Hence, the EIGTHRESH (see below) variable should be used to set the point of singular value truncation. To achieve this, set MAXSING to a number equal to, or greater than, the maximum number of estimable parameters. This is the best setting to use in most cases.

- **EIGTHRESH** is the eigenvalue ratio threshold for truncation (0 ≤ EIGTHRESH < 1). To ensure numerical stability of the inversion process this should be set to 5E-7 or above, for this is the value at which numerical noise can be amplified to a level where it
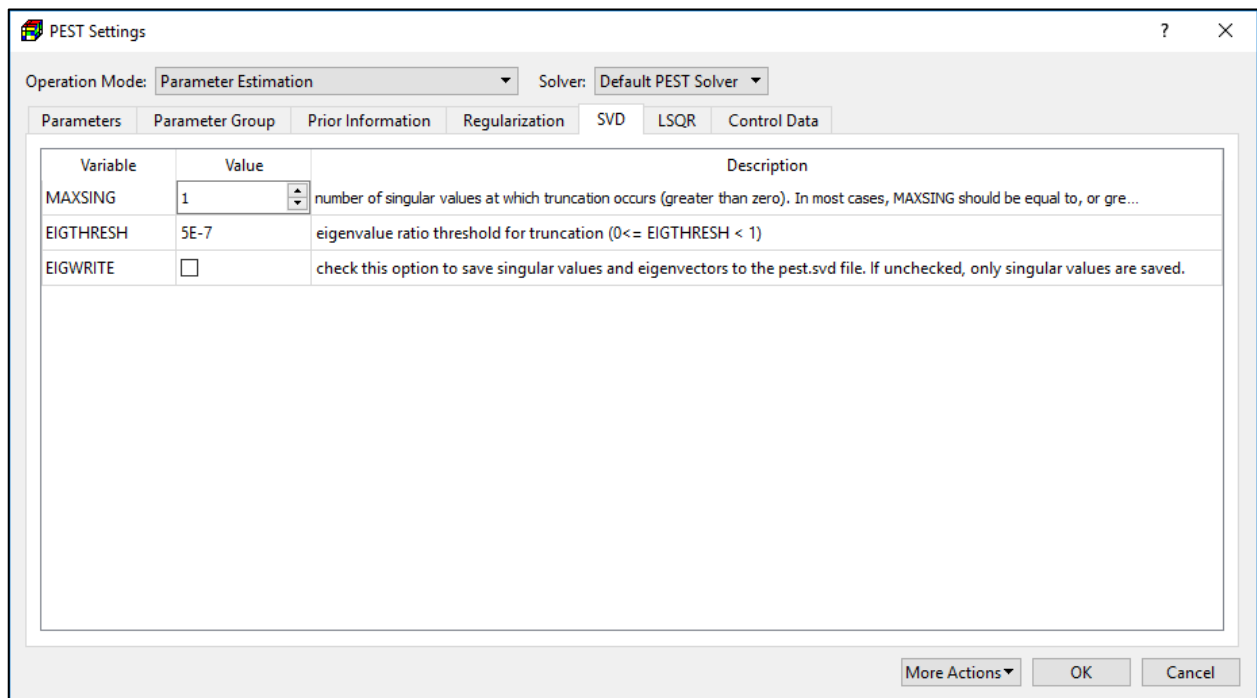
Figure 112. The SVD tab of the PEST Settings dialog box

smothers the "signal" contained in the calibration dataset. See Section 4.4 of the Part I of the PEST Manual (Doherty, 2016) for details.

- **EIGWRITE:** Check this option to save singular values and eigenvectors to the SVD output file pest.svd. If unchecked, only singular values are saved. The SVD output file can become very large and not all the information recorded in this file is always worth reading. However sometimes an inspection of singular values can assist in understanding the degree to which an inverse problem is ill-posed.

9. **LSQR Tab** (Figure 113)**:** The variables of this tab are used only if the Solver is LSQR.

- **LSQR_ATOL:** This is the LSQR *atol* input variable and must be zero or greater. This variable is defined as "*An estimate of the relative error in the data defining the matrix **A**. For example, if **A** is accurate to about 6 digits, set atol to 1.0e-6.*"

- **LSQR_BTOL:** This is the LSQR *btol* input variable and must be zero or greater. This variable is defined as "*An estimate of the relative error in the data defining the rhs vector **b**. For example, if **b** is accurate to about 6 digits, set btol to 1.0e-6.*"

- **LSQR_CONLIM:** This is the LSQR *conlim* input variable and must be zero or greater. A value of 1000.0 generally works well with PEST. See Section 4.5.2 of the Part I of the PEST Manual (Doherty, 2016) for the definition of *conlim*.

- **LSQR_ITNLIM:** This is the LSQR *itnlim* input variable and must be greater than 0. This value should be set to four times the number of adjustable parameters as recommended by (Doherty, 2016).
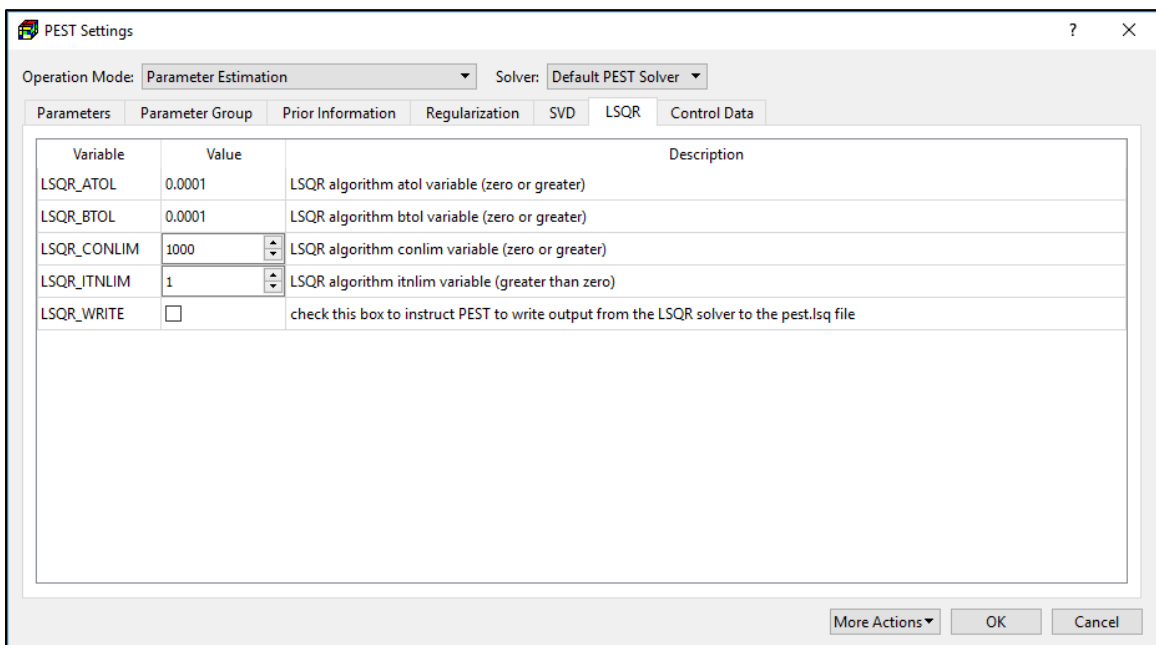
Figure 113. The LSQR tab of the PEST Settings dialog box

- **LSQR_WRITE:** Check this box to instruct PEST to write output from the LSQR solver to the pest.lsq file. Information from each LSQR call is appended to this file; hence it can become quite lengthy.

10. **Control Data Tab** (Figure 114)**:** This section provides a brief explanation of the control data. For detailed discussion, see Section 4.2 of the Part I of the PEST Manual (Doherty, 2016).

- **PRECIS** defines the format for writing parameter values to model input files.

- **DPOINT**: Select *nopoint* to omit decimal point from representations of parameter values on model input files. Select *point* to ensure that the decimal point is always present.

- **RLAMBDA1** is the value of initial Marquardt lambda and must be zero or greater. A value of 10.0 is appropriate in most cases. However, if PEST complains about the normal matrix being singular you may need to raise it.

- **RLAMFAC** is the factor by which PEST adjusts the Marquardt lambda. RLAMFAC must be greater than 1.0; a value of 2.0 seems to work well on many occasions. When PEST reduces lambda, it divides by RLAMFAC; when it increases lambda, it multiplies by RLAMFAC.

- **PHIRATSUF** is the fractional objective function sufficient for end of current iteration. PHIRATSUF must be between 0 and 1. A value of 0.3 is appropriate in most cases. During an iteration of the inversion process, PEST may calculate a parameter upgrade vector using several different Marquardt lambdas. First it lowers lambda and, if this is unsuccessful in lowering the objective function, it then raises lambda. If, at any stage, it calculates an objective function which is a fraction PHIRATSUF or less of the starting

Figure 114. The Control Data tab of the PEST Settings dialog box

objective function for that iteration, PEST considers that the goal of the current iteration has been achieved and moves on to the next iteration.

- **PHIREDLAM** is the termination criterion for Marquardt lambda search. PHIREDLAM must be between 0 and 1. If the relative reduction in the objective function between the use of two consecutive lambdas is less than PHIREDLAM, PEST moves to the next iteration.

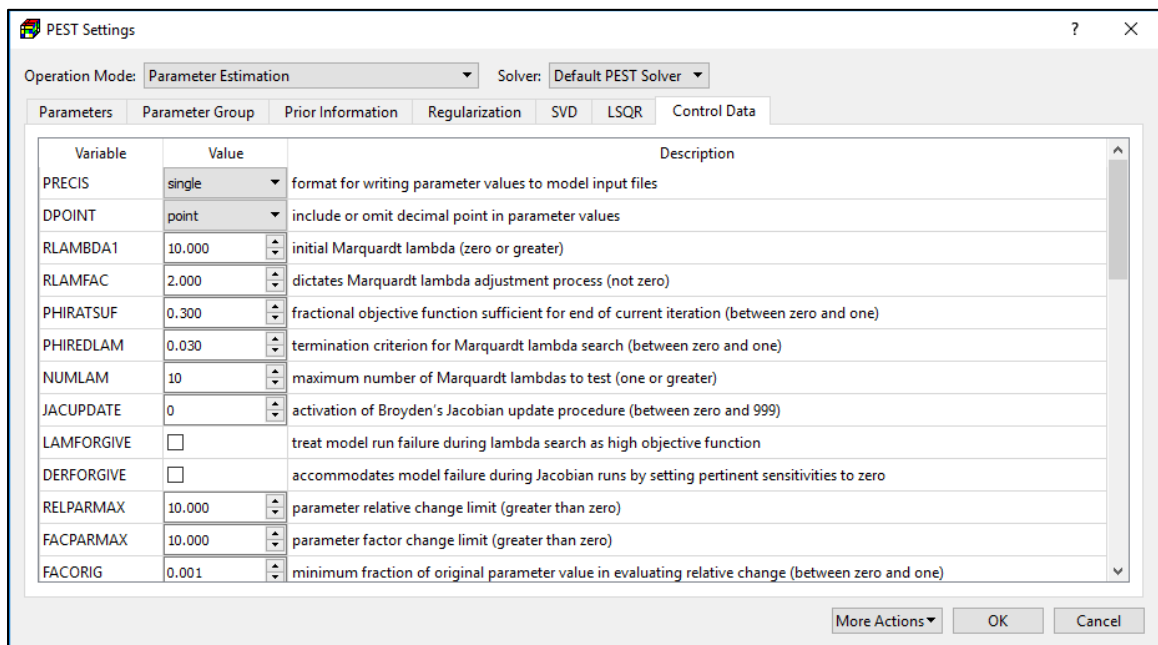- **NUMLAM** is the maximum number of Marquardt lambdas to test during an iteration. NUMLAM must be 1 or greater and should normally be set to 10.

- **JACUPDATE** is used in conjunction with the activation of Broyden's Jacobian update procedure, which provides a mechanism for improving the Jacobian matrix based on model outputs calculated during model runs undertaken for testing parameter upgrades calculated using different values of the Marquardt lambda.

  o If it is set to zero, Broyden updating of the Jacobian matrix does not occur.
  o If it is set to 999, Jacobian matrix is updated after the first parameter upgrade attempt, and every parameter upgrade attempt thereafter.
  o If it is set to n, where 0 < n < 999, Broyden updating will be undertaken during a PEST iteration following the first *n* attempts to upgrade parameters using *n* different values of the Marquardt lambdas.

- **LAMFORGIVE** treats model run failure during lambda search as high objective function.

  o If this box is unchecked: when a model fails to run to completion during a parameter estimation process, PEST reports this error condition and ceases execution with an error message.
  o If this box is checked: when a model fails to run to completion during a parameter estimation process, PEST ignores the failed model run and attempts new sets of parameters using other values of the Marquardt lambda. If it failed to find parameters that allow the model to complete execution, PEST either switches to central derivatives calculation or ceases execution with an appropriate error message.

- **DERFORGIVE** plays a similar role to LAMFORGIVE. However, DERFORGIVE governs PEST's behavior when model runs are being undertaken for finite-difference derivatives calculation. If this box is checked, DERFORGIVE accommodates model failure during Jacobian runs by setting pertinent sensitivities to zero.

- **RELPARMAX** is the maximum relative change that a parameter may undergo between optimization iterations. RELPARMAX must be greater than zero.

- **FACPARMAX** is the maximum factor change that a parameter may undergo between optimization iterations. FACPARMAX must be greater than zero.

- **FACORIG**: If the absolute value of a parameter falls below FACORIG times its original value, then FACORIG times its original value is used in evaluating relative change. FACORIG is not used to adjust limits for log-transformed parameters. FACORIG must be greater than zero. A value of 0.001 is often suitable.

- **IBOUNDSTICK** instructs PEST not to compute derivatives for parameter hits its bounds for the given number of times.

- **UPVECBEND**: If this box is checked, PEST will bend the parameter upgrade vector if a parameter hits its bounds. Normally, this box should be unchecked.

- **PHIREDSWH**: If FORCEN (see Parameter Group Tab above) is set to "switch" or "switch_5", and if the relative reduction in the objective function between successive iterations is less than the PHIREDSWH, PEST will switch from single to three-point or five-point derivatives calculation. A value of 0.1 is often suitable for PHIREDSWH.

- **NOPTSWITCH** is the iteration before which PEST will not switch to higher order derivatives computation. NOPTSWITCH must be one or greater. A value of 3 or 4 often works well. If in doubt, set the value to 1.

- **SPLITSWH** determines when, in the inversion process, split slope analysis begins. split slope analysis will begin when the ratio of the best objective function achieved during a certain iteration to that achieved in the previous iteration is equal to or higher than SPLITSWH. If SPLITSWH is provided with a zero or negative value it is ignored. Normally, SPLITSWH should be set to zero, even if split slope analysis is activated.

- **DOAUI**: Check this box to instruct PEST to implement automatic user intervention. Only on very rare occasions is automatic user intervention useful. Insensitivity of one or a number of parameters is accommodated far more gracefully using singular value decomposition or LSQR as a solution device for the inverse problem.

- **DOSENREUSE**: Check this box to instruct PEST to reuse parameter sensitivities. On most occasions, there is little benefit to be gained from invoking PEST's sensitivity reuse functionality. For details, see Section 7 of the Part I of the PEST Manual.

- **BOUNDSCALE**: If this box is checked, parameters are scaled by the inter-bounds interval if using SVD or LSQR as the solver. Experience has shown that on most occasions scaling by bounds is worth a try.

- **NOPTMAX** is the maximum number of optimization iterations and must be -2 or greater.
  - If NOPTMAX is set to 0, PEST will not estimate parameters, nor even calculate a Jacobian matrix. Instead it will terminate execution after just one model run. This setting can be used to ensure that PEST setup is correct; at the same time, it can be used to compute objective function components and residuals based on initial parameter values.

o If NOPTMAX is set to -2 PEST will calculate the Jacobian matrix, store it in the pest.jco file, and then cease execution immediately. This matrix can then be used for linear analysis, and/or for construction of an SVD-assist input dataset.

o Setting NOPTMAX to -1 instructs PEST to compute the Jacobian matrix. However, after doing this, PEST records the same information on its output files as that which it would normally record on completion of an inversion process. This includes composite sensitivities and, if pertinent, post-calibration uncertainty and covariance statistics calculated from parameter sensitivities. It then undertakes a final model run so that model input and output files remaining after PEST execution is complete pertain to parameters values provided in the PEST control file.

- **PHIREDSTP** and **NPHISTP**: PHIREDSTP is the relative objective function reduction triggering termination and must be greater than zero. NPHISTP is the number of successive iterations over which PHIREDSTP applies. For many cases 0.005 and 4 are suitable values for PHIREDSTP and NPHISTP respectively.

- **NPHINORED**: If PEST has failed to lower the objective function over NPHINORED successive iterations, it will terminate execution. A value of 3 or 4 is often suitable.

- **RELPARSTP** and **NRELPAR**: If the magnitude of the maximum relative parameter change between iterations is less than RELPARSTP over NRELPAR successive iterations, PEST will cease execution. A value of 0.005 is often suitable for RELPARSTP. A value of 3 or 4 is normally satisfactory for NRELPAR.

- **PHISTOPTHRESH**: If PHISTOPTHRESH is set to a positive number, PEST will cease execution if the objective function falls below this value at the end of any iteration. If PHISTOPTHRESH is set to zero or a negative number, then it is ignored.

- **LASTRUN**: Check this box to instruct PEST to undertake (or not) final model run with best parameters.

- **PHIABANDON** is the objective function value at which to abandon optimization process. Set this to a very high number or to a non-positive number to deactivate this function.

- **ICOV, ICOR,** and **IEIG**: If PEST is run in "estimation" mode, and if the Default PEST Solver is used in solution of the inverse problem, then at the end of each iteration of the inversion process PEST can write linear estimates of the posterior covariance and correlation coefficient matrices, as well as eigenvectors and eigenvalues of the posterior covariance matrix to the pest.mtt file. Check the boxes of ICOV, ICOR and IEIG to enable the output of the respective matrices.

- **IRES:** Check this box to instruct PEST to record resolution data to the pest.rsd file. This is a binary file which is used by utilities such as RESPROC, RESWRIT and PARAMERR which compute the resolution matrix, and quantify post-calibration predictive error variance.

- **JCOSAVE:** Check this box to instruct PEST to save best Jacobian file as the pest.jco file.

- **VERBOSEREC:** Check this box to instruct PEST to include parameter and observation data lists in the run record file. Uncheck this box so that PEST will write a much shorter run record file.

- **JCOSAVEITN**: Check this box to instruct PEST to write current Jacobian matrix to iteration-specific pest.jco.n file at the end of every optimization iteration, where n is the number of iteration.

- **REISAVEITN**: Check this box to instruct PEST to store best-fit residuals to iteration-specific residuals files pest.rei.n at end of every optimization iteration, where n is the iteration number.

- **PARSAVEITN:** Check this box to instruct PEST to store iteration specific parameter value files pest.par.n at end of every optimization iteration, where n is the iteration number.

- **PARSAVEITN:** Check this box to instruct PEST to creates a series of run specific parameter value files named pest.par.n_m where n is the run packet index and m is the run number within that packet. For identification purposes, run packet indices are also recorded on the run management record file pest.rmr. This file also records run numbers and the nodes to which runs were allocated. Hence a user can associate parameter values with the runs performed by different nodes involved in PEST parallelization.

3.8.4.2. Run

Select this menu item to open the Run PEST dialog box (Figure 115). It can be used to start the parameter estimation process with PEST, to build input files to MODFLOW and PEST, or to check the model data. The settings of this dialog box are described below.
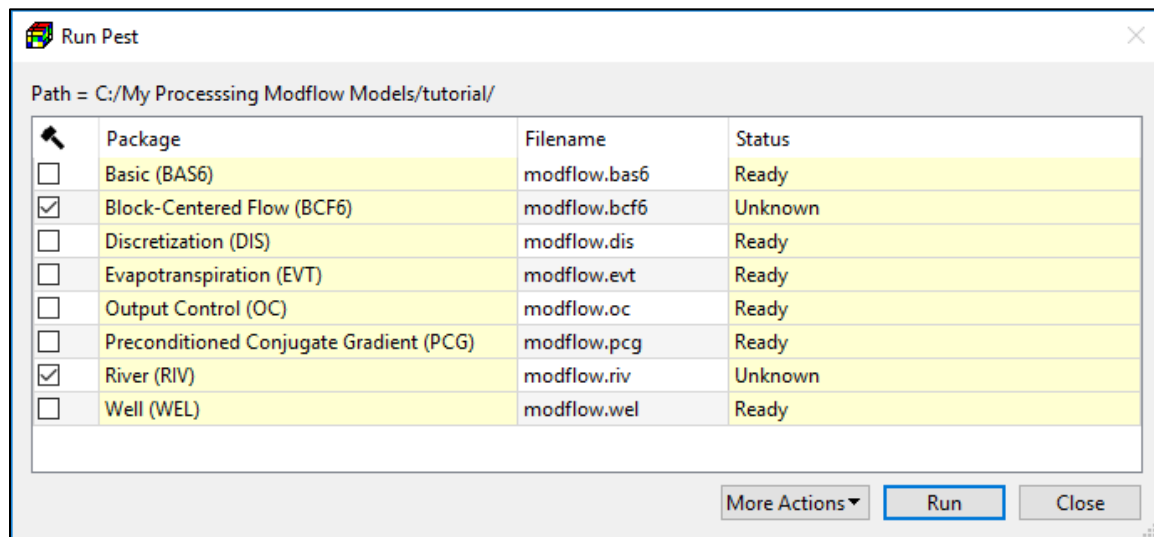

Figure 115. The Run Pest dialog box

1. **Table**

   - ⚒ **The build box.** Prior to running PEST or BeoPEST, PM uses the user-specified data to build input files for MODFLOW and template files for PEST. An input file (and its template file, if applicable) will be built if its build box is checked. If an input file does not exist or the input data has been modified since the last build, its build box will be checked automatically. A template file of a package is needed for PEST, if the package contains estimable parameters.

   - **Package** is the name of the package of the flow model.

   - **Filename** is the name of the input file to MODFLOW. The base filename of the corresponding template file to PEST is "pest", instead of "modflow".

   - **Status** shows the status (such as Ready, Not Exist, etc.) of the input file.

2. **More Actions**

   - **Inspect Model Data:** Select this to check the geometry of the model and the consistency of the model data. Table 3 shows a list of items that are inspected by PM. The inspection report will be saved in the *modflow_inspection_log.txt* file.

   - **Build Input Files:** Select this to build the input files (and template files, if applicable) with the checked build boxes. The name file modflow.nam and input file modflow.lmt for LMT8 package will also be built. In addition, several batch files (*.bat) are also created for PEST and/or BeoPEST. Consult the build log files, *modflow_build_log.txt* and pest_*build_log.txt* for details. These files are in the model data folder.

   - **Rebuild All Input Files:** Select this to rebuild all input files, except for existing input files that are marked as read-only.

3. **Run:** Click this button to build input files (and their template files) with the checked build boxes and the start the parameter estimation process. The following rules apply.

   - If *PEST Version* (in the Preferences dialog box) is "Standard PEST", the estimation process will be carried out by the executable file of PEST defined in the Preferences dialog box (Figure 26). If *PEST Version* is "BeoPEST", the estimation process will be carried out by the executable file of BeoPEST defined in the Preferences dialog box (Figure 26).

   - If LPF or BCF is selected as the internal flow package, the flow simulation will be carried out by the executable file of MODFLOW-2005 defined in the Preferences dialog box (Figure 26). If UPW is selected as the internal flow package, the flow simulation will be carried out by the executable file of MODFLOW-NWT defined in the Preferences dialog box (Figure 26).

   The PEST or BeoPEST run progress will be displayed in the PEST Output window. You may terminate the process at any time by clicking on the Terminate button.

3.8.4.3. Run PESTCHEK

Select this menu item to check for the correctness and consistency of the PEST control file built by PM. PESTCHEK may provide additional advices beyond data checking. Running PESTCHEK is normally not necessary, if the PEST or BeoPEST software that comes with PM are used.

3.8.4.4. View

The View menu allows you to display several output files of PEST. These files are briefly described below. For detailed discussions, refer to Part I of the PEST Manual (Doherty, 2016).

3.8.4.4.1. Run Record File

As PEST executes, it writes a detailed record of the parameter estimation process to the run record file pest.rec. if the parameters and/or observations are large in number this file can get very long. In that case, you should uncheck VERBOSEREC box in the Control Data Tab of the PEST Settings dialog box.

3.8.4.4.2. Estimated Parameter Values

At the end optimization-iteration, PEST writes the best parameter set achieved so far (i.e., the set for which the objective function is lowest) to the parameter file pest.par. The first line of the file contains the values for the character variables PRECIS and DPOINT, which were used in the PEST control file. Then follows a line for each parameter, each line containing a parameter name, its current value and the values of the SCALE and OFFSET variables for that parameter. Using values from intermediate parameter-estimation iterations, that are likely to be closer to the optimal parameter values, often reduces execution time.

3.8.4.4.3. Residuals

On completion of parameter estimation process, PEST writes a "residuals file" tabulating observation names, the groups to which observations belong, measured and modelled observation values, differences between these two (i.e. residuals), measured and modelled observation values multiplied by respective weights, weighted residuals, measurement standard deviations and "natural weights". This file can be readily imported into a spreadsheet for various types of analysis and plotting. The name of the residuals file is pest.res.

3.8.4.4.4. Interim Residuals

At the beginning of each iteration PEST writes the interim residuals file pest.rei. It contains six columns of data. The first two columns cite observation names and group names; then follow observation values and their current model-generated counterparts. Current residuals and weights follow that in subsequent columns.

3.8.4.4.5. Composite Parameter Sensitivities

Immediately after it calculates the Jacobian matrix, PEST writes composite parameter sensitivities to the parameter sensitivity file pest.sen. The information contained in this file allows you to track variations in the composite sensitivity of each parameter through the parameter estimation process.

3.8.4.4.6. Composite Observation Sensitivities

The Observation Sensitivity file pest.seo contains all observation values and corresponding model-calculated values, as well as composite sensitivities for all observations. The composite sensitivity of an observation is a measure of the sensitivity of that observation to all parameters involved in the parameter estimation process. A high value of composite observation sensitivity normally indicates that an observation is particularly crucial to the inversion process.

3.8.4.4.7. SVD Output File

When SVD is activated, PEST writes the SVD output file pest.svd in addition to other output files. The SVD output file can become very large and not all the information recorded in this file is always worth reading. However sometimes an inspection of singular values can assist in understanding the degree to which an inverse problem is ill-posed.

3.8.4.4.8. Scatter Chart

To display the scatter chart based on the head data, select *Scatter Chart > Head*. To display the scatter chart based on the drawdown data, select *Scatter Chart > Drawdown*. For details, see Section 3.8.1.5.3.

3.8.4.4.9. Line Chart

To display the line chart based on the head data, select *Line Chart > Head*. To display the line chart based on the drawdown data, select *Line Chart > Drawdown*. For details, see Section 3.8.1.5.4.

Chapter 4. Visualization and Postprocessing

This chapter describes how to visualize and postprocess the input/output data of the active model. The item of the active model on the TOC contains two major groups, namely Input Data and Visualization. The former can be used to adjust visualization settings of the input data, including model grid, flow packages, and observation points. The latter may include many types of items, such as input parameter contours, simulation result contours, flow vectors, and pathlines via MODPATH instances.

As mentioned in Chapter 1, each of these items on the TOC represents a map layer that contains a visual representation of the item's data. The available visualization settings of the active layer are displayed in the Settings window. This chapter discusses these visualization settings.

4.1. Input Data

4.1.1. Model Grid

As shown in Figure 116, the display settings of the model grid are organized in several groups based on the nature of the data. These settings are described below. By right-clicking on the *Model Grid* item and selecting *Export to Shapefile*, you can export the shapefiles of the individual groups to a zip file.

1. **General**

   - **Display Layer**: This is the layer number of the model grid. When multiple items are displayed on the Map Viewer, the items with smaller layer numbers are displayed on top of the items with larger layer numbers.

2. **Model Bounding Box**

   - **Visible:** Check this box to turn on the display of the model bounding box encompassing all cells of the model.

   - **Opacity**: The model box is opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.
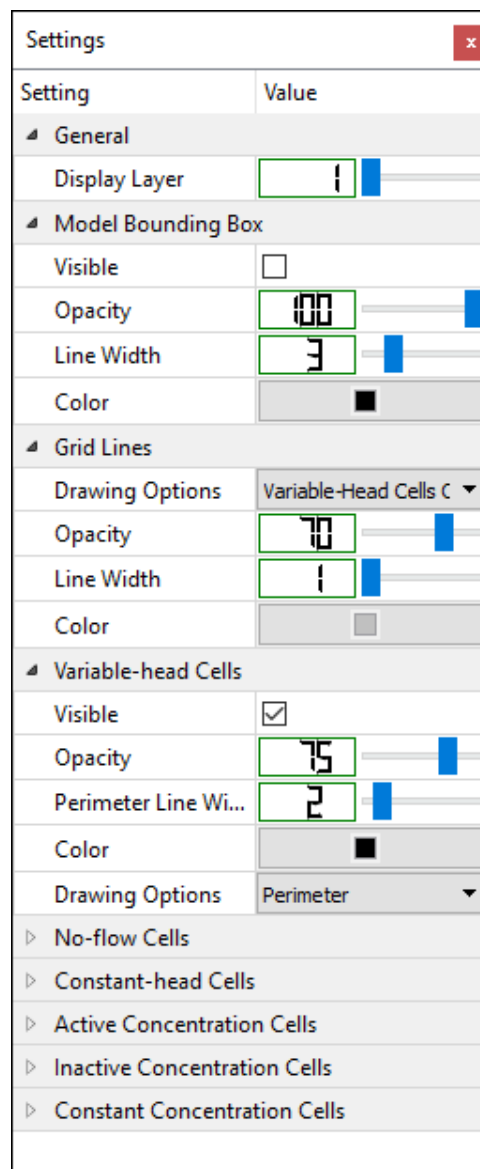

Figure 116. The Settings window for model grid

- **Line Width** is the line width (in pixels) that is used to draw the model box.
- **Color:** Use this dropdown box to select a color for the model box.

3. **Grid Lines**
   - **Drawing Options**
     - o **Do Not Draw**: The grid lines will not be displayed.
     - o **All Cells**: The grid lines of all cell types will be displayed.
     - o **Variable-Head Cells Only**: The grid lines of variable-head cells will be displayed.
     - o **No-Flow Cells Only:** The grid lines of no-flow cells will be displayed.
   - **Opacity**: The grid lines are opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.
   - **Line Width** is the line width (in pixels) that is used to draw the grid lines.
   - **Color:** Use this dropdown box to select a color for the grid lines.

4. **Variable-head Cells, No-flow Cells, Dry Cells** [45] **, Constant-head Cells, Active Concentration Cells, Inactive Concentration Cells, Fixed Concentration Cells:** The available settings of these groups are the same. Use them to adjust the display settings of the respective cell types.
   - **Visible**: Check this box to display the cells.
   - **Opacity**: The cells or their perimeter is opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.
   - **Perimeter Line Width** is the line width (in pixels) that is used to draw the perimeter of the cells. This value is used only if the Drawing Option (see below) is *Perimeter.*
   - **Color**: Use this dropdown box to select a color for the cells or their perimeter.
   - **Drawing Options**
     - o **Color Filled:** If this option is selected, all cells will be filled with the color selected by the Color dropdown box.
     - o **Perimeter:** If this option is selected, the perimeter of the cells will be drawn with the line width and color defined in *Perimeter Line Width* and *Color*.

4.1.2. Packages

Each item in this group corresponds to an item in the *Models > Modflow > Packages* menu. By right-clicking on an item in this group, you have access to the following options:

1. **Export to Shapefile**: this will export the package to a shapefile.

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[45] Dry Cells are the model cells that went dry during a flow simulation. The hydraulic head result file modflow.head file is required for Dry Cells to work.

2. **Remove Package**[46]: this option removes the package and erases its data.

3. **Deactivate Package**[46]: this option deactivates the package but retains its data. A deactivated package may be activated by selecting the corresponding item in the *Models > Modflow > Packages* menu.

Each package has a Display Setting group in the Settings window. The following display settings are common among packages.

1. **Display Layer**: This is the layer number of the package. When multiple map layers are displayed, the layers with smaller layer numbers are displayed on top of the layers with larger layer numbers.

2. **Opacity**: The cells of the package is opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.

3. **Color**: Use this dropdown box to select a color for the cells of the package. Note that some packages have several color boxes. For example, the Well Package has separate color boxes for pumping, injection, and inactive wells.

4. **Highlight Parameter:** Within the Data Editor, you can double-click on a cell to highlight all other cells that have the same cell value as the clicked cell. The cell values of the selected Highlight Parameter will be used for this purpose.

4.1.3. Observation Points

By right-clicking on an item in this group, you can display a popup menu that allows you to edit, import, or export observation points and data. For details, see Section 3.5.3. The visualization settings of the observation points (Figure 117) are as follows:

1. **General**
   - **Display Layer:** This is the layer number of the Observation Points. When multiple items are displayed, the items with smaller layer numbers are displayed on top of the items with larger layer numbers.

2. **Observation Point**
   - **Draggable** determines whether the observation points may be dragged by the mouse.
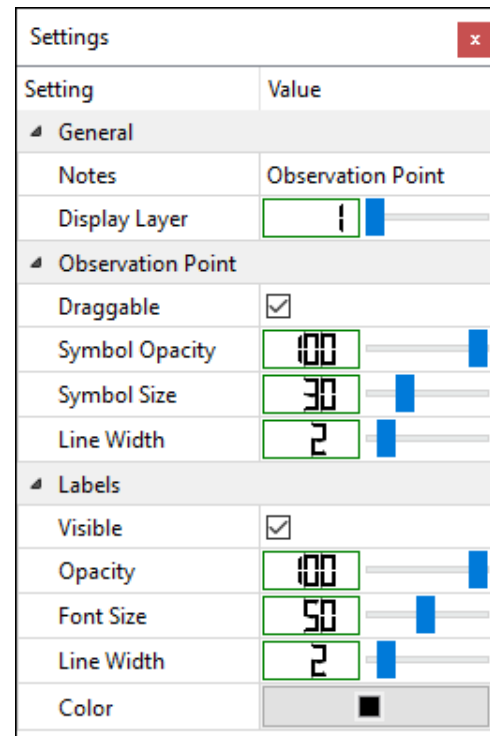   - **Symbol Opacity:** The observation points are opaque if the value of opacity is 100,

Figure 117. The Settings window for observation points

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[46] This option is available only when the package is not being edited.

translucent if the value is between 1 and 99, and transparent if the value is 0.

- **Symbol Size** defines the size of the observation point.
- **Line Width** is the line width (in pixels) that is used to draw the observation points.

3. **Labels** defines the properties of observation point labels.
   - **Visible:** Check this box to display the labels of the observation points.
   - **Opacity:** The labels are opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.
   - **Font Size** defines the size of the labels.
   - **Line Width** is the line width (in pixels) that is used to draw the labels.
   - **Color:** Use this dropdown box to select a color for the labels.

4.2. Visualization

4.2.1. Input Parameter Contours

4.2.1.1. Create Contour Maps Based on Input Parameters

You can create contour maps based on the cell-by-cell values of model input parameters by right-clicking on Input Parameter Contours on the TOC, select *Add* from a popup menu, and then select an input parameter from the Select Data dialog box. The following input parameters are supported:

1. Data entered through the Discretization and Parameters menus.
2. MODFLOW: Evapotranspiration (EVT), Evapotranspiration Segments (ETS), Recharge (RCH), as well as Subsidence and Aquifer-Compaction Packages.
3. MT3D: Dispersion (DSP), Reaction (RCT), and Sink & Source Mixing (SSM) Packages.
4. SEAWAT: Prescribed fluid density and prescribed dynamic viscosity.

After adding a Contour Map item to the TOC, you can right-click on the item to access the following functions:

1. **Show All Items**: the contour map contains several items, one for each contour level. Select this to display all contour levels.
2. **Hide All Items:** Select this to hide all contour levels.
3. **Export to Shapefile:** this will display the Save As dialog box where you can select a shapefile (with the extension .shp) for storing the contour map.
4. **Export Matrix Data:** Select this to open the Export Data dialog box (see Figure 35 on page 58 for details).
5. **Remove Item**: Select this to remove the Contour Map item.

4.2.1.2. Customize Contour Maps

The visualization settings of the input parameter contour map are as follows:

1. **General** (Figure 118)

   - **Name:** The text string is the name of the Contour Map displayed on the TOC.

   - **Notes:** The text string can be used for notes.

   - **Reference** may be either None or one of the following parameters: Sand Box 1, Sand Box 2, Sand Box 3, Starting Head, Top of Layer, and Bottom of Layer.

     - If None is selected, the cell values are used for constructing the contour map,
     - Contours will not be created for the areas with the reference value equals to -1E20. You can crop out an area by assigning -1E20 to the cells within that area,
     - If the *Invert Reference* box is checked, the results of "reference - cell values" are used for constructing the contour map. If the *Invert Reference* box is cleared, the results of "cell values – reference" are used for

     Figure 118. The General group of the Settings window for Contour Maps

     constructing the contour map. You can, for example, create a contour map of layer thickness by selecting Top of Layer as the input parameter and using Bottom of Layer as the Reference.

   - **Invert Reference:** Check the box to invert the reference (see *Reference* above).
   - **Display Layer:** This is the layer number of the contour map. When multiple items are displayed, the items with smaller layer numbers are displayed on top of the items with larger layer numbers.

   - **Resolution** determines the maximum number of values that are used for contouring. The available options with the corresponding maximum number of values are listed below. It is recommended to use a lower resolution when trying out various settings.

     - **Native**: Use the native model resolution.
     - **Highest**: 150,000.
     - **High**: 112,500
     - **Medium**: 75,000.
     - **Low**: 37,500.
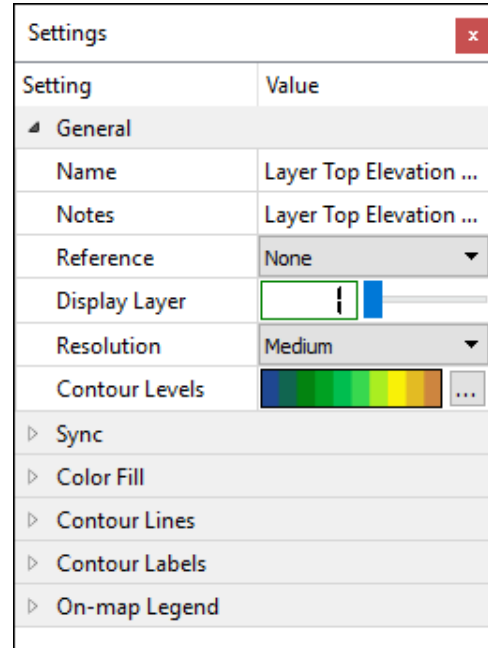   - **Lowest**: 5,000.

Before a matrix of the input parameter values (the matrix) is used for contouring, the matrix may be refined or down-sampled to match the selected resolution according to the following rules.

o For contours on the Map Viewer, the following rules apply to the matrix:

– If a model has only one row or one column, the matrix at its native resolution is used.

– If a model has more than one row and one column, the matrix is either refined (by inserting values between cells and estimating those values by linear interpolation based on nearby cell values) or down-sampled to match the selected resolution.

o For contours on the Cross-section window:

– If a model has only one layer, the matrix at its native resolution is used.

– If a model has more than one layer,

▪ if the native resolution is selected or if the selected resolution is lower than the native resolution, the matrix at its native resolution is used. Contours will not be displayed in the parts of the model where only one layer is active.

▪ if the selected resolution is higher than the native resolution, the matrix is refined by inserting values on the top/bottom of model and between cell centers. Those values are estimated by linear interpolation using up to four values of surrounding cells. The inserted values on the top or bottom of the model are estimated by linear interpolation using up to two values of surrounding cells in the top or bottom layers, respectively.

- **Contour Levels:** The contour levels can be defined by clicking on the [...] button to open the Classes dialog box (Figure 119).

  o **Color-Mapping Table:** The table displays the colors and corresponding parameter values. The default values of the table are based on the minimum and maximum values of all cells. Cell values, that are equal to -1E20, less than the first row or greater than the last row, are not used for contouring. When displaying color-filled
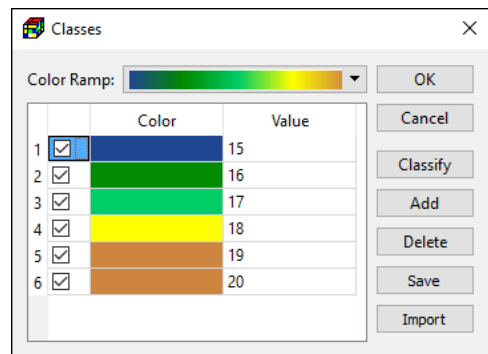
Figure 119. The Classes dialog box

contours, the color of a row is used to fill the area between the contour levels of the given row and the next row.

  o **Color Ramp:** Select a predefined color ramp from this dropdown box to assign graduated colors to the color-mapping table.

o **Classify**: Click this button open the Classify dialog box (Figure 120) that is used to define the range of values and number of classes. If *Min. Value* and *Max. Value* are both positive, the option of *Use logarithmic scale between Min and Max Values* is available. Click the Default button to reset *Min. Value and Max. Value* to the values found in the data of the current layer.

Figure 120. The Classify dialog box

o **Add** is used to add a contour level to the table. Click this button to open the Add Value dialog box, where a new contour can be entered.

o **Delete**: To delete a contour level, first click on the desired row on the table, then click this button.

o **Save**: Click this button to save the color-mapping table in an XML file.

o **Import**: Click this button to import a saved XML file to the color-mapping table.

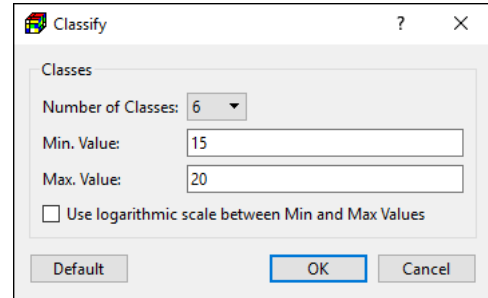2. **Sync** (Figure 121)**:** The settings of this group control what data is displayed.

• **Mode**

o **Auto**: The stress period, layer, species controls are deactivated and synced with the corresponding controls on the toolbar. The contour map will be updated accordingly, whenever any of the controls on the toolbar is changed or if the values of the input parameter are modified by using *Tools > Data > Modify or Tools > Data > Import*.

o **Lock**: The stress period, layer, species controls are deactivated and locked at their current settings. The contour map will never change, even if the values of the input parameter are modified.

Figure 121. The Sync group of the Settings window for Contour Maps

o **Manual:** The stress period, layer, species controls are activated when applicable. The contour map will be updated accordingly, whenever any of these controls is changed or if the values of the input parameter are modified by using *Tools > Data > Modify* or *Tools > Data > Import*.
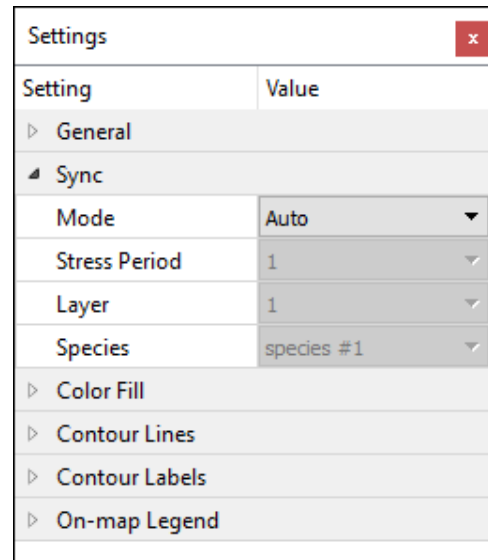
• **Stress Period:** For time-independent model data, such as HK or T, this control is deactivated and is not used. For time-dependent model data, such as Recharge Flux,

the data of the selected stress period is displayed. For transient sand boxes the following rules apply:

o If the Mode is Auto, contour maps are created based on the matrix values that are linearly interpolated from the nearby stress periods to the time point at the end of the selected stress period and time step (on the toolbar). When running an animation process, the contour map is created for individual time frames.

o If the Mode is Manual, contour maps are created based on the matrix values that are linearly interpolated from the nearby stress periods to the time point at the end of the stress period defined by this control.

- **Layer:** For layer-dependent model data (such as HK), the data of the selected layer is displayed. For layer-independent model data (such as Maximum EVT Flux), this control is deactivated and is not used.

- **Species:** For species-dependent model data (such as initial concentration), the data of the selected layer is displayed. For species-independent model data (such as HK), this control is deactivated and is not used.

3. **Color Fill** (Figure 122)

- **Visible:** Check this box to fill the contours with the colors defined in the color-mapping table.

- **Opacity:** The color-fill is opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.

4. **Contour Lines** (Figure 123)

- **Visible:** Check this box to display the contour lines.

- **Opacity:** The contour lines are opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.

- **Line Width** is the line width (in pixels) that is used to draw the contour lines.

- **Color:** Use this dropdown box to select a color for the contour lines.

Figure 122. The Color Fill group of the Settings window for Contour Maps
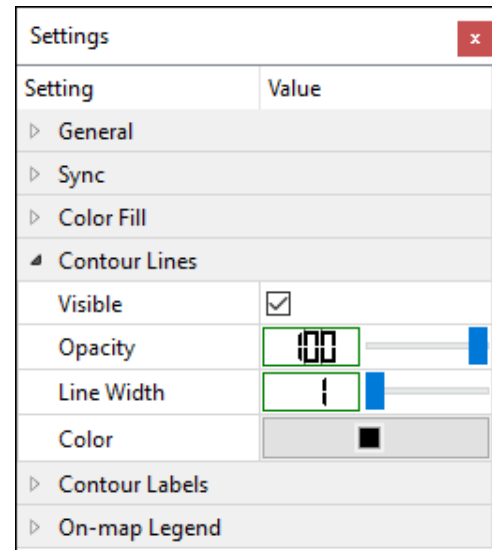
Figure 123. The Contour Lines group of the Settings window for Contour Maps

5. **Contour Labels** (Figure 124)

- **Visible:** Check this box to display the contour labels.

- **Opacity:** The contour labels are opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.

- **Distance** controls the distance between contour labels. A smaller number yields more labels.

- **Font Size** controls the font size of the contour labels.

- **Line Width** is the line width (in pixels) that is used to draw the contour labels.

- **Color:** Use this dropdown box to select a color for the contour labels.

- **Format**
    - **Decimal Notation** formats values in the form [-]9.9.
    - **Scientific Notation** formats values in the form [-]9.9E[±]999.
    - **Compact Notation** uses the decimal or scientific notation, whichever is the most concise.

- **Precision:**
    - For Decimal and Scientific Notations: maximum number of digits after the decimal point
    - For Compact Notation: maximum number of significant digits.

6. **On-map Legend** (Figure 125)

- **Visible:** Check this box to display the on-map legend.

- **Opacity:** The legend is opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.

- **Width:** This defines the relative width of the legend. The larger the number the wider is the legend.
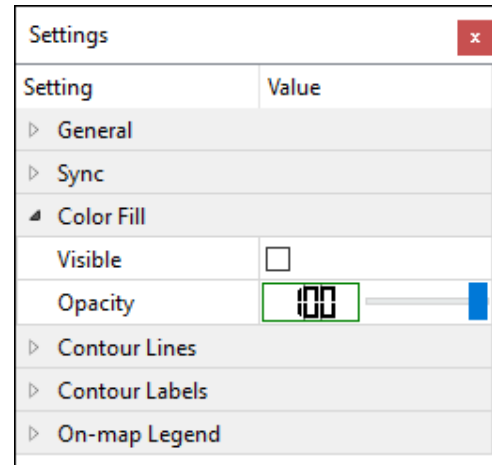
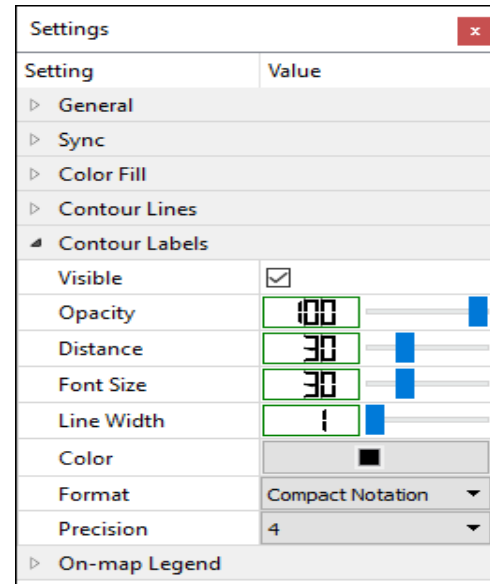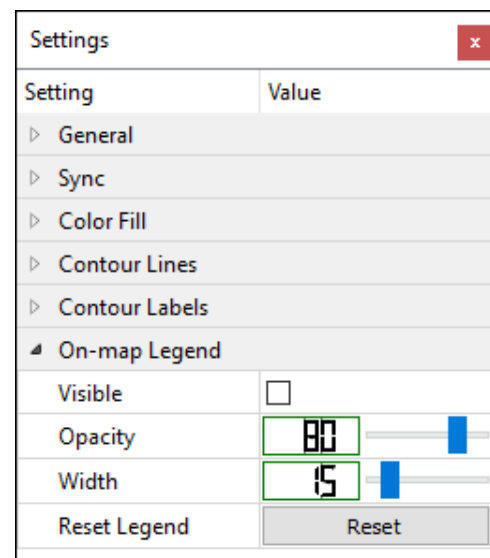*Figure 124. The Contour Labels group of the Settings window for Contour Maps*

Figure 125. The On-map Legend group of the Settings window for Contour Maps

- **Reset Legend:** Click the Reset button to reset the legend to its default size and position.

4.2.2. Result Contours

4.2.2.1.   Create Contour Maps Based on Model Results

You can create a contour map based on the model result data by right-clicking on Result Contours on the TOC, select *Add* from a popup menu, and then select a data type from the Select Data dialog box. Contours will not be created for the areas of no-flow or dry cells, or areas with the reference value (see Reference in Section 4.2.1.2 above) equals to -1E20. In addition, the areas of inactive concentration cells will be omitted for concentration contours.

The following cell-by-cell model result data types are supported:

1. **Hydraulic head:** the default output file "modflow.head" in the model folder will be used.
2. **Drawdown:** the default output file "modflow.drawdown" in the model folder will be used.
3. **Concentration:** You need to select a result file of MT3D from the Open File dialog box. The default file names of the result files are MT3Dnnn.UCN for the dissolved phase and MT3Dnnns.UCN for the sorbed phases, where nnn is the species number.
4. **Cell-By-Cell Flow Terms:** the default output file "modflow.flow" in the model folder will be used. The following supported data types are stored in that file: Storage, Interbed Storage, Constant Head, Drains, Drains with Return Flow, General-Head Boundary, River Leakage, Stream Leakage, Stream Flow Out, Evapotranspiration, Evapotranspiration Segments, Recharge, Flow Right Face, Flow Front Face, Flow Lower Face, Horizontal Flux (flux at the cell center based on fluxes across the horizontal cell faces), Vertical flux (flux at the cell center based on fluxes across the top and bottom cell faces), Flux (flux at the cell center based on fluxes across all cell faces).
5. **Interbed Storage Package:** the default output file "modflow.interbed" in the model folder will be used. The following supported data types are stored in that file: Subsidence, Compaction, and Critical Head.
6. **Seawater Intrusion 2 Package:**
   - The calculated interface elevation (Zeta surface elevation) are stored in the output file "modflow.swi2zeta". On the Map Viewer, the calculated zeta surface elevation may be used to create contour maps. On the cross-section window, the position of the zeta surface is marked with open circles (see Figure 126 for an example.) The display settings of the markers can be adjusted with the controls in *Zeta Marker on Cross Section* group of the Settings window.
   - The other supported data types are stored in the "modflow.flow" file: Flow Right Face Correction, Flow Lower Face Correction, Flow Front Face Correction, and Constant Head Flow Correction. These correction terms are intended to be added to the corresponding cell-by-cell flow terms to yield the final flow results.
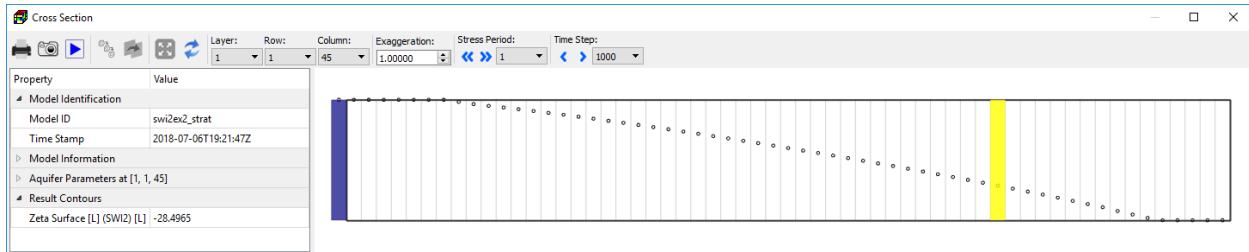
Figure 126. The position of zeta surface is marked with open circles on the cross section

After adding a Contour Map item to the TOC, you can right-click on the item to access the following functions:

1. **Show All Items**: the contour map contains several items, one for each contour level. Select this to display all contour levels.

2. **Hide All Items:** Select this to hide all contour levels.

3. **Export to Shapefile:** this will display the Save As dialog box where you can select a shapefile (with the extension .shp) for storing the contour map.

4. **Export Matrix Data:** Select this to open the Export Data dialog box that allows you to export the matrix data of the displayed results. See Figure 35 on page 58 for details about the dialog box.

5. **Set as Starting Head:** if the contour map is based on the calculated hydraulic head, this item allows you to set the calculated hydraulic head values (of all layers) as the starting hydraulic head values. For dry cells, the starting hydraulic head values are set to the cell bottom elevations. This feature is useful if you plan to run a transient flow model with the starting hydraulic head values based on the results of a prior model.

6. **Remove Item**: Select this to remove the Contour Map item.

4.2.2.2.   Customize Contour Maps

Most of the visualization settings of a result contour map are the same as those described in Section 4.2.1.2. The following is a list containing the result-contour specific settings:

1. **General**
   - **Result File** is the (read-only) name of the binary file that contains the cell-by-cell model result values. Refer to Section 0 for the output file names of the supported models.

2. **Sync**
   - **Mode**
     o **Auto**: The controls of the Sync group are deactivated and synced with the corresponding controls on the toolbar. Whenever the model is run, or any of the corresponding controls on the toolbar is changed, the contour map will be updated with the most recent model results.

o **Lock**: The stress period, layer, date/time, and output times controls are deactivated and locked at their current settings. The contour map will never change, even if the model results have changed.

o **Manual:** The stress period, layer, date/time, and output times controls are activated when applicable. The contour map will be based on the model results of the date/time defined by the Date/Time control.

- **Date/Time** is the date/time for which the model result is displayed.

  o If the selected Mode is Auto, Date/Time will be set to the end of the stress period and time step defined on the toolbar.

  o If the selected Mode is Manual, you may edit the date/time. After editing of the date/time is finished[47], the values for Stress Period and Time Step will update accordingly and the contour map will be updated with "model result – reference" at the given date/time.

- **Output Times:** This is available for concentration contours. The dropdown box contains the output times that are found in the selected concentration file. When an item of the Output Times dropdown box is selected, the value for the Date/Time control will be set to the selected item and the contour map will be updated with "model result – reference" at the given date/time.

- **Stress Period** and **Time Step:** When the stress period or time step is changed, the value for the Date/Time control will be set to the end of the given stress period and time step. The contour map will be updated with "model result – reference" at the given date/time.

- **Layer:** This is the model layer for which the "model result – reference" is displayed on the Map Viewer. This control does not affect the display on the Row Cross Section tool.

3. **Potentiometric Surface on Cross Section:** This group appears only if the result data type is Hydraulic Head. The potentiometric surface on a vertical column of model cells is defined as the hydraulic head at the highest active cell. The potentiometric surface on a cross section is formed by linking the potentiometric surface of individual vertical columns. The following settings define the appearance of the potentiometric surface on the model cross-section.

- **Visible:** Check this box to display the potentiometric surface on the cross-section window.

- **Opacity:** The potentiometric surface is opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.

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[47] Editing is finished when the Date/Time control loses focus or when enter is pressed.

- **Line Width:** This is the line width (in pixels) that is used to draw the potentiometric surface.

- **Color:** Use this dropdown box to select a color for the potentiometric surface.

4. **Zeta Marker on Cross Section:** This group appears only if the result data type is Zeta Surface. The settings define the appearance of the markers that mark the position of the zeta surface on the model cross-section.

- **Visible:** Check this box to display the zeta markers on the cross-section window.

- **Opacity:** The markers are opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.

- **Line Width:** This is the line width (in pixels) that is used to draw the markers.

- **Size:** This defines size of the zeta markers.

- **Color:** Use this dropdown box to select a color for the zeta markers.

4.2.3. Flow Vectors

You can create flow vectors for individual cells by right-clicking on this item and then select *Add* from a popup menu. Flow vectors are based on the computed cell-by-cell flow terms[48], head values, effective porosity, and the geometry of the cells. The following input parameters are supported:

1. **General** (Figure 127)

    - **Name:** The text string is the name of the Flow Vectors Map displayed on the TOC.

    - **Notes:** The text string can be used for notes.

    - **Display Layer:** This is the layer number of the contour map. When multiple items are displayed, the items with smaller layer numbers are displayed on top of the items with larger layer numbers.

    - **Popup on Hover:** If this is checked, when the mouse cursor hovers over a vector, a popup window containing detailed data of the vector will be displayed.

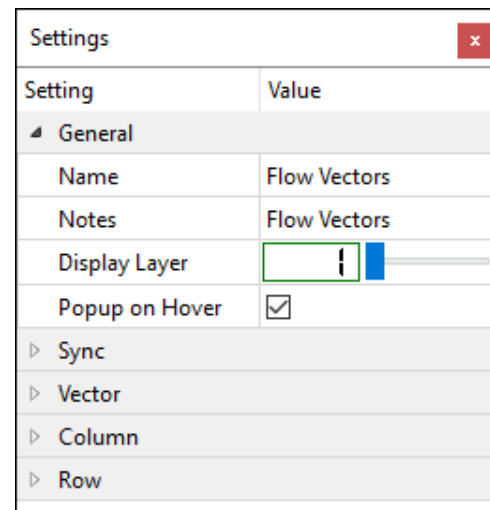*Figure 127. The General group of the Settings window for Flow Vectors*

2. **Sync** (Figure 128)

    - **Mode**

        o **Auto**: The stress period, time step and layer controls are deactivated and synced with the corresponding controls on the toolbar. Whenever the model is run or any

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[48] Flow correction terms from the SWI2 package are included in the calculation and display of flow vectors.

of the controls is changed, the contour map will be updated based on the most recent model results.

- o **Lock**: The stress period, layer, species controls are deactivated and locked at their current settings. The contour map will never change, even if the model results have changed.

- o **Manual:** The stress period, layer, species controls are activated when applicable. The contour map will be created based on the model results of the specified stress period, time step, and species when applicable.

Figure 128. The Sync group of the Settings window for Flow Vectors

- **Date/Time** is the date/time for which the model result is displayed. After editing of the date/time is finished, the values for Stress Period and Time Step will update accordingly and the flow vectors will be updated with the model result at the given date/time.

- **Stress Period** and **Time Step:** When the stress period or time step is changed, the value for the Date/Time control will be set to the end of the given stress period and time step. The flow vectors will be updated with model result at the given date/time.

- **Layer:** This is the model layer for which the flow vectors are displayed.

3. **Vector** (Figure 129)

- **Opacity:** The flow vectors are opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.

- **Line Width** is the line width (in pixels) that is used to draw the flow vectors.

- **Color:** Use this dropdown box to select a color for the flow vectors.

- **Data Type:**

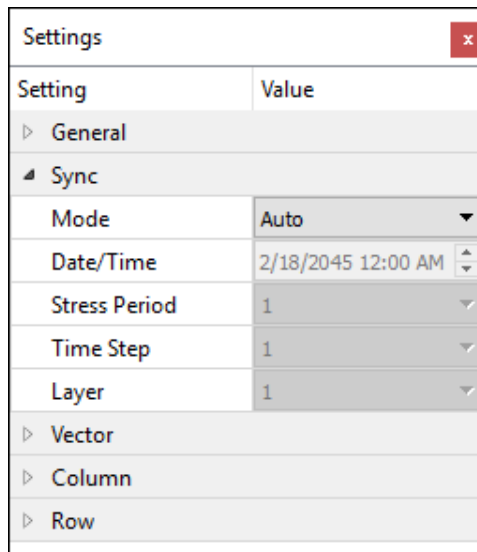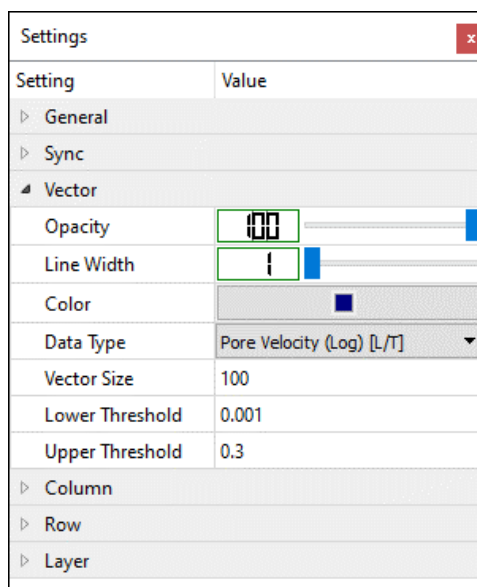- o **Volumetric Flow Rate [L^3T^{-1}]:** The flow vectors are scaled by groundwater flow rate.

Figure 129. The Vector group of the Settings window for Flow Vectors

o **Volumetric Flow Rate (Log) [L³T⁻¹]:** The flow vectors are scaled by logarithmic value of groundwater flow rate.

o **Darcy Velocity [LT⁻¹]:** The flow vectors are scaled by the Darcy velocity.

o **Darcy Velocity (Log) [LT⁻¹]:** The flow vectors are scaled by logarithmic value of the Darcy velocity of groundwater.

o **Pore Velocity [LT⁻¹]:** The flow vectors are scaled by the pore velocity which is equal to Darcy velocity divided by the effective porosity.

o **Pore Velocity (Log) [LT⁻¹]:** The flow vectors are scaled by logarithmic value of the pore velocity.

- **Vector Size** is a scale factor of the display length of flow vectors. The display length of a vector is determined based on its magnitude of the selected Data Type and Upper Threshold (see below).

- **Lower Threshold** and **Upper Threshold:** A flow vector is displayed only if its magnitude is between the lower threshold (inclusive) and the upper threshold (inclusive). Assign zero or a negative value to deactivate a threshold. The default values of the Lower and Upper thresholds are the respective minimum and maximum values of pore velocity of the current time step and stress period.

o If Upper Threshold is equal to or less than zero, the display length of a vector is scaled between 0 and the highest magnitude of the selected Data Type in the current flow field. That is, the flow vectors of different model layers or simulation times may be scaled differently.

o If Upper Threshold is greater than zero, the display length of a vector is scaled between 0 and Upper Threshold. If you need to compare flow vectors of different model layers or simulation times, assign a positive value to Upper Threshold (and a positive value to Lower Threshold, if the selected Data Type involves log-transformed values).

4. **Column, Row,** and **Layer** (Figure 130)**:** The values of these groups define the region of interest. Only the flow vectors that lie within the region of interest are displayed. The Interval values specify how often the vectors should be displayed. For example, if start row is 5, end row is 16, and the row interval is 3, then the vectors at the rows 5, 8, 11, and 14 are displayed. The values of the Layer group only apply to the vectors on the Row Cross

Settings		
Setting	Value	
▷ General		
▷ Sync		
▷ Vector		
◢ Column		
Start	1	
End	60	
Interval	1	
◢ Row		
Start	1	
End	1	
Interval	1	
◢ Layer		
Start	1	
End	1	
Interval	1	

Figure 130. The Column and Row groups of the Settings window for Flow Vectors

Section Window or Column Cross Section Window. The values of the Column and Row groups only apply to the vectors on the Map Viewer.

4.2.4. MODPATH[49] Instances

4.2.4.1. Create MODPATH Instances

You can create a MODPATH instance by right-clicking on *MODPATH* on TOC and then select *Add* from a popup menu. An item, named *Instance*, will be added to the MODPATH group. You can right-click on the MODPATH instance to access the following functions:

1. **Remove Item**: This will remove the MODPATH instance.
2. **Delete All Starting Points**: Delete all particles (starting points).
3. **Import Starting Points**: this will display the Open File dialog box where you can select a file that contains the starting points (particles) data. See Section 5.1.6 for the format of the MODPATH Starting Points file.
4. **Export Starting Points**: this will display the Save As dialog box where you can select a file for exporting starting points (particles) data to. See Section 5.1.6 for the format of the MODPATH Starting Points file.
5. **Export to Shapefile**: this will display the Save As dialog box where you can select a ZIP file for storing the exported the results of MODPATH to shapefiles, including pathlines, starting points, end points, and time marks.

4.2.4.2. Time Concepts

MODPATH uses the following time concepts. The terms defined below are expressed in the model time unit.

1. **Simulation Time** is the elapsed time since the start of the MODFLOW simulation. Simulation time starts at 0 and increases throughout the course of a MODFLOW simulation.
2. **Reference Time** is a specified point of Simulation Time that marks the beginning of a MODPATH particle tracking simulation.
3. **Tracking Time**: This is the elapsed time relative to Reference Time. Tracking time is 0 at Reference Time. Tracking time measures the accumulated time during a particle-tracking analysis. The value of tracking time is always positive, regardless of whether particles are tracked in the forward or backward direction.

4.2.4.3. Add Particles

In MODPATH, particles (starting points) may be released at different time points. The release time of a particle is defined based on the settings when the particle is added to the map. For forward tracking, the release time of new particles is set to the beginning of the current time step and stress period. For backward tracking, the release time is set to the end of the current time

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[49] MODPATH does not account for the cell-by-cell flow correction terms of SWI2.

step and stress period. Once particles are added to the map, their release times, start locations, and display colors are fixed.

There are two ways to add particles.

1. **Add Individual Particles**

   - Click the MODPATH instance to make it the active layer and the click on the MODPATH Tool button ⊹ on the toolbar.

   - Modify the *Tracking Direction* and the settings of the *Particle Start Point* group of the MODPATH instance as needed. See Section 4.2.4.5 for details.

   - Move to the layer, where the particles should be placed.

   - Click the mouse at the desire location on the map to add a particle. The vertical coordinate of the particle is defined by $z = z_{bot} + z_L \cdot (z_{top} - z_{bot})$, where z_{bot} and z_{top} are the elevations of layer bottom and top, respectively, and z_L is the local vertical coordinate defined by Local Z (see Figure 134) in the settings window.

2. **Add a Group of Particles**

   - Click the MODPATH instance to make it the active layer and then click on the MODPATH Tool button ⊹ on the toolbar.

   - Modify the *Tracking Direction* and the settings of the *Particle Start Point* group of the MODPATH instance as needed. See Section 4.2.4.5 for details.

   - Move to the layer, where the particles should be placed.

   - Click and drag the mouse cursor to draw a box covering the region where particles should be placed, then release the mouse button to open the Add Particles dialog box (Figure 131).

   - Using the Add Particles dialog box, you can place particles on faces of the cells, within the cells, or on circles centered at the cells that are located inside the drawn box. The features of this dialog box are as follows

     o **Particle Color** is the color for new particles. To change a color, click on the ⊡ button and then pick a color from the Select Color dialog box.

     o **Particles on cell faces:** Check the box
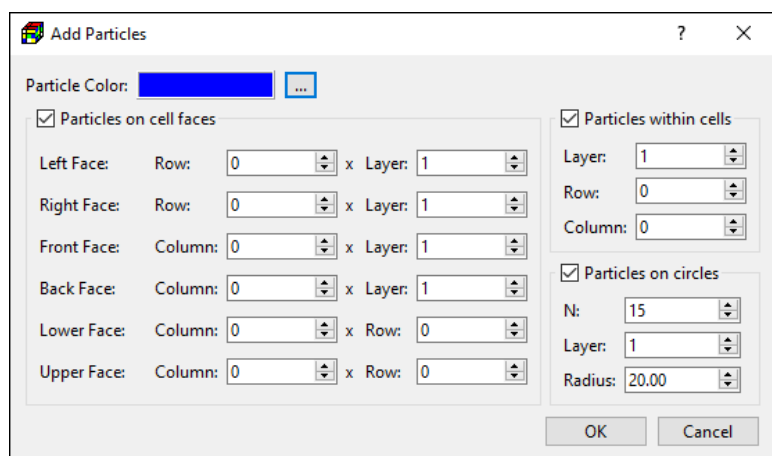
Figure 131. The Add Particles dialog box

to activate this group. It controls the number of particles that will be placed on the faces of the cells that are located inside the drawn box. The number of particles on each face is equal to the product of the respective specified numbers.

o **Particles within cells:** Check the box to activate this group. It controls the number of particles that will be placed within the cells that are located inside the drawn box. The number of particles for each cell is equal to the product of the specified values for *Layer*, *Row,* and *Column*.

o **Particles on circles:** Check the box to activate this group. It controls the number of particles that will be placed on circles centered at the cells that are located inside the drawn box. *N* is the number of particles on a circle, *Layer* is the number of circles in the vertical direction, and *Radius* is the circle radius.

4.2.4.4. Delete Particles

1. **Delete Particles of a Layer**

- Click the MODPATH instance to make it the active layer and the click on the MODPATH Tool button ⌖ on the toolbar.

- Move to the layer, where the particles should be deleted.

- Press and hold the Shift-key and the left mouse button, move the mouse to drag a box encompassing the particles that should be deleted, and then release the Shift-key and left mouse button.

2. **Delete Particles of all Layers**

- Click the MODPATH instance to make it the active layer and the click on the MODPATH Tool button ⌖ on the toolbar.

- Press and hold the Control-key and the left mouse button, move the mouse to drag a box encompassing the particles that should be deleted, and then release the Control-key and left mouse button.

4.2.4.5. Customize MODPATH Settings

1. **General** (Figure 132)

- **Name:** The text string is the name of the MODPATH instance displayed on the TOC.

- **Notes:** The text string can be used for notes.

- **Display Layer:** This is the layer number of the particles, time marks, and pathlines. When multiple items are displayed, the items with smaller layer numbers are displayed on top of the items with larger layer numbers.

- **Popup on Hover:** If this is checked and when the mouse cursor hovers over an object, such as a particle, time mark, or pathline, a popup window containing detailed data of the object will be displayed and the corresponding pathline will be highlighted.

- **Highlight Pathline:** If this is checked and when the mouse cursor hovers over an object, such as a particle or time mark, highlight the pathline containing that object.

- **Instance ID:** This is the unique identifier of the MODPATH instance. The base filename of the input and output files of this MODPATH instance is MODPATH-*InstanceID*.

- **Time Stamp:** This is the time stamp (in UTC) of the last MODPATH run.

2. **Particle Tracking** (Figure 133)

- **MODPATH**: Click the *Run* button to build input files to MODPATH and then start MODPATH. The run progress will be displayed in the MODPATH Output window. You may terminate the run at any time by clicking on the Terminate button. After completing the MODPATH run, the pathlines and time point markers will be displayed automatically.

- **Number of Time Points** is the number of time points at which the locations of particles should be saved in an output file.

- **Time Point Interval** is the interval of time (expressed in the model time unit) between time points. A Time Point Marker is placed whenever the *Tracking Time* is a multiple of the given Time Point Interval.

- **Tracking Direction** defines whether the simulation tracks particles forward or backward in time. The tracking direction affects the release time of particles.

  - **Forward**: When particles are added to the map, their release time is the beginning of the current stress period/time step.
  - **Backward**: When particles are added to the model, their release time is the end of the current stress period/time step. Thus, if you want to simulate backward particle tracking from the end of the flow
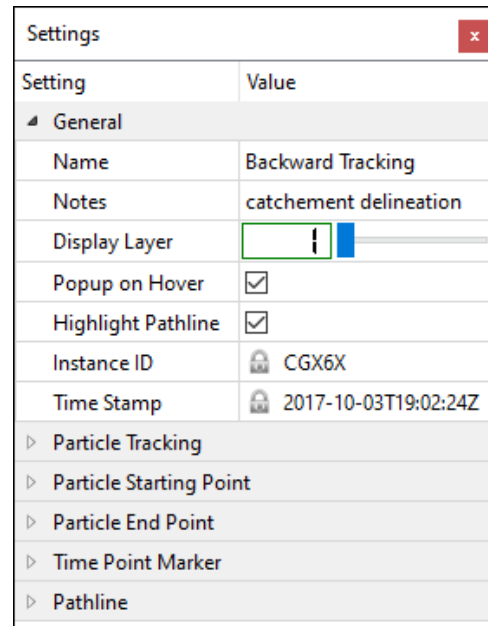

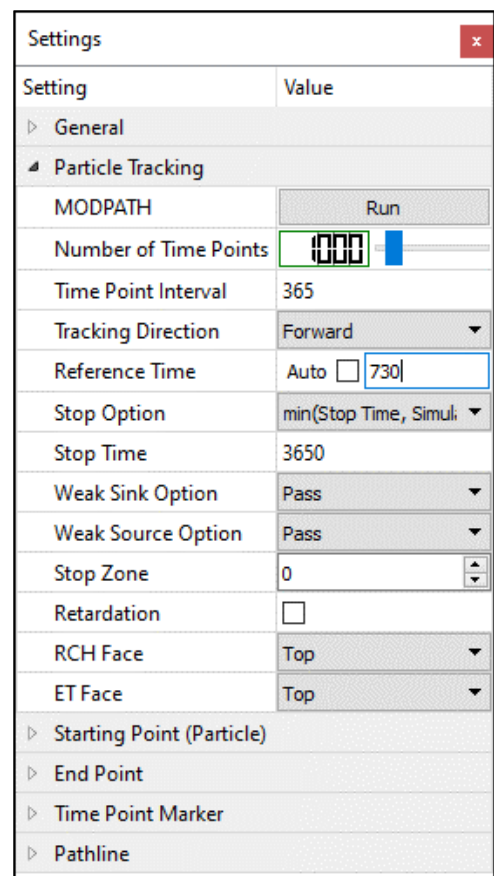*Figure 132. The General group of the Settings window for MODPATH*

Figure 133. The Particle Tracking group of the Settings window for MODPATH

simulation, you need to choose this setting and set the stress period/time step to the last ones, before adding new particles.

- **Reference Time** is a specified point of Simulation Time that marks the beginning of a MODPATH particle tracking simulation. If the **Auto** box is checked, *Reference Time* is to 0 (start of the flow simulation) for forward particle tracking and is set to *Simulation Length* (end of the flow simulation) for backward particle tracking.

- **Stop Option:**

  o **Simulation Limit:**

  – For forward tracking, stop the particle tracking simulation at the end the final time step of the MODFLOW simulation.

  – For backward tracking, stop the particle tracking simulation at the beginning of the MODFLOW simulation.

  o **Extended**:

  – For forward tracking, extend the final steady-state time step (if applicable) and track all particles until they reach termination locations.

  – For backward tracking, extend the initial steady-state time step (if applicable) and track all particles until they reach termination locations.

  o **min(Stop Time, Simulation Limit):** Particles are stopped when the *Stop Time* (see below) or Simulation Limit is reached.

- **Stop Time** is the *Tracking Time* at which a particle tracking simulation is stopped. Stop Time is used only if the selected Stop Option is *min(Stop Time, Simulation Limit).*

  Simply put, a forward particle tracking simulation stops at the simulation time equal to [*Reference Time + Stop Time*]. A backward particle tracking simulation stops at the simulation time equal to [*Reference Time – Stop Time*]. For example, assuming you have a flow model with the simulation length of 1000. Setting *Stop Time* to 300 and *Reference Time* to 100 will stop a forward particle tracking at the simulation time 100 + 300. Setting *Stop Time* to 300 and *Reference Time* to 900 will stop a backward particle tracking at the simulation time 900 – 300.

- **Weak Sink Option** defines whether particles should be stopped when they enter weak sink cells or should pass through weak sink cells. A strong sink cell is one that contains an internal sink and has inflow from adjacent cells but no outflow to other cells. In contrast, weak sink cells have both inflow and outflow across their cell faces.

- **Weak Source Option** defines whether particles should be stopped when they enter weak source cells or should pass through weak source cells. A strong source cell is one that contains an internal source and has outflow to adjacent cells but no inflow from other cells. In contrast, weak source cells have both inflow and outflow across their cell faces.

- **Stop Zone:** A value greater than zero activates the Stop Zone option of MODPATH. A value of zero deactivate the Stop Zone option. When the Stop Zone option is activated, particles will stop when entering cells with the same stop zone value as given here. Use *Parameters > Stop Zone* to assign stop zone values to cells.

- **Retardation:** The travel velocity of a particle is set to its pore velocity divided by Retardation. Particles move slower with a larger Retardation value. The retardation values are defined by *Parameters > Retardation Factor* with the Data Editor.

- **RCH Face:** recharge may be treated as a distributed source or assigned to a cell face by selecting a corresponding option.

- **ET Face:** evapotranspiration may be treated as a distributed sink or assigned to a cell face by selecting a corresponding option.

3. **Particle Starting Point** (Figure 134)

   - **Opacity:** The particle starting points are opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.

   - **Size:** This defines the display size of all particle starting points.

   - **Color:** Use this dropdown box to select a color for new particles that are added to the map individually as described in Section 4.2.4.3.

   - **Local Z:** This is the local z coordinate of new particles that are added to the map individually as described in Section 4.2.4.3.

4. **Particle End Point** (Figure 134): particle end points are displayed as diamonds on the map viewer, and they represent the particle stop locations.

   - **Opacity:** The particle end points are opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.

   - **Size:** This defines the display size of the particle end points.

   - **Color:** Use this dropdown box to select a color for the particle end points.

5. **Time Point Marker** (Figure 134)

   - **Opacity:** The time point markers are opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.
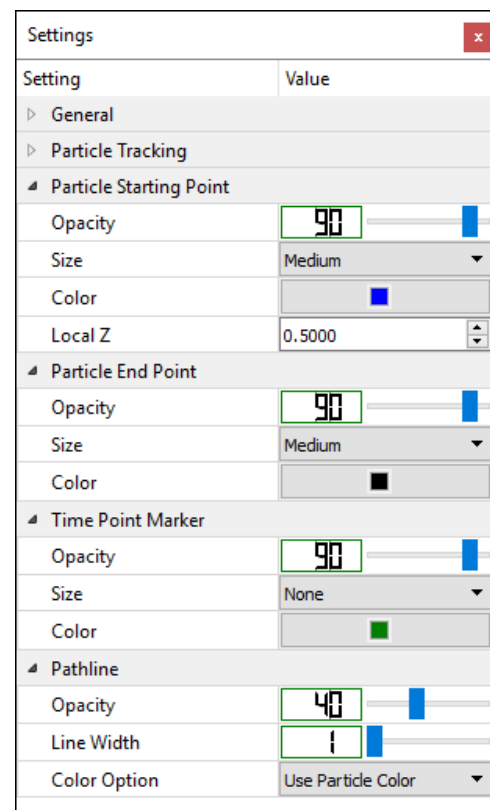
Figure 134. The Particle Starting Point, Particle End Point, Time Point Marker, and Pathline groups of the Settings window for MODPATH

- **Size:** This defines the display size of the time point markers.

- **Color:** Use this dropdown box to select a color for the time point markers.

6. **Pathline** (Figure 134)

- **Opacity:** The pathlines are opaque if the value of opacity is 100, translucent if the value is between 1 and 99, and transparent if the value is 0.

- **Line Width** is the line width (in pixels) that is used to draw the pathlines.

- **Color Option**

  o Use Particle Color: Pathlines are displayed in the same color as the respective particle starting points.

  o Use Layer Color: Pathlines are displayed in the color of the corresponding layer where the pathlines are located. The layer colors are defined in the Layer Property dialog box. See Section 3.6.3 for details.

Chapter 5. Supplementary Information

5.1. File Formats

5.1.1. 2D Matrix and 2D Weight Matrix

A 2D Matrix or 2D Weight Matrix file is a text file with the following format that can be exported from or imported to the Data Editor as described in Section 3.5.19.

File Format
1. #2DMATRIX
2. NCOL, NROW
3. MATRIX

Description

- **#2DMATRIX:** The first line holds the text string "#2DMATRIX" that serves as the file format identifier.

- **NCOL, NOW** are, respectively, the numbers of columns and rows of the matrix that follows.

- **MATRIX** is a two-dimensional data matrix saved row by row. The data of the first model row is given on the first row of the file, the second follows, and so on. Each row contains NCOL values from left to the right. The values must be separated by a space or comma.

Example

The following is an example showing a 2D Matrix file for a grid with 4 columns and 3 rows. The grid values are representing by a 4 x 3 matrix.

```
#2DMATRIX
4, 3
11, 12, 34, 23
42, 35, 23, 21
23, 41, 31, 19
```

5.1.2. 2D Modflow Array

A 2D Modflow Array file is a text file with the following format that can be exported from or imported to the Data Editor as described in Section 3.5.19.

File Format
1. #2DMODFLOWARRAY
2. NCOL, NROW
3. ARRAY

Description

- **#2DMODFLOWARRAY:** The first line holds the text string "#2DMODFLOWARRAY" that serves as the file format identifier.

- **NCOL, NOW** are, respectively, the numbers of columns, and rows of the array that follows.

- **ARRAY** is a two-dimensional data array saved in the format as described in the section "Input Instructions for Array Reading Utility Subroutines" of Chapter 8 in (Harbaugh, 2005). Note that arrays saved in external binary files are not supported.

Example

The following is an example showing a 2D Modflow Array file for a grid with 4 columns and 3 rows. The grid values are representing by a 4 x 3 matrix.

```
#2DMODFLOWARRAY
4, 3
INTERNAL 1 (FREE) -1
11, 12, 34, 23
42, 35, 23, 21
23, 41, 31, 19
```

The following is an example showing a 2D Modflow Array file for a grid with 9 columns and 7 rows. The grid has a constant value of 526.

```
#2DMODFLOWARRAY
9, 7
Constant 526
```

5.1.3. 3D Modflow Array

A 3D Modflow Array file is a text file with the following format that can be exported from or imported to the Data Editor as described in Section 3.5.19.

File Format
1. #3DMODFLOWARRAY
2. NCOL, NROW, NLAY

   (the following array repeats NLAY times)
3. ARRAY

Description

- **#3DMODFLOWARRAY:** The first line holds the text string "#3DMODFLOWARRAY" that serves as the file format identifier.

- **NCOL, NOW** are, respectively, the numbers of columns and rows of the arrays that follows.

- **NLAY** is the number of occurrences of the ARRAY saved in this file.

- **ARRAY** is a two-dimensional data array saved in the format as described in the section "Input Instructions for Array Reading Utility Subroutines" of Chapter 8 in (Harbaugh, 2005). Note that arrays saved in external binary files are not supported. ARRAY is repeated NLAY times. The first occurrence of the array is for the first (top) model layer, the second occurrence for the second layer, and so on. If NLAY is greater than the number of model layers, only the first occurrences that are equal to the number of model layers are used.

Example

The following is an example showing a 3D Modflow Array file for a grid with 4 columns, 3 rows, and 2 layers. For the first layer, the grid values are representing by a 4 x 3 matrix. For the second layer, the grid has a constant value of 37.

```
#3DMODFLOWARRAY
4, 3, 2
INTERNAL 1 (FREE) -1
11, 12, 34, 23
42, 35, 23, 21
23, 41, 31, 19
Constant 37
```

5.1.4. Comma-Separated Values File

A Comma-Separated Values file is a text file with the following format that can be exported from or imported to the Data Editor as described in Section 3.5.19.

File Format
1. #CSV
2. X, Y, Z (repeat this line as many times as needed)

Description

- **#CSV:** The first line holds the text string "#CSV" that serves as the file format identifier.

- **X, Y, Z:** Each line represents a data point, where [x, y] are the coordinates of the point, and z is the value at the point. If an optional prj file[3] exists in the same folder as the CSV file, [x, y] are expressed in the coordinate system defined by the prj file. If a prj file does not exists, [x, y] are assumed to be [longitude, latitude], where longitude and latitude are expressed in WGS84.

5.1.5. ASCII Raster

ASCII Raster, also known as ASC/INFO ASCII GRID, is a non-proprietary raster GIS file format developed by ESRI. ASCII Raster files may be exported or imported via the Data Editor, see

Section 3.5.19 for details. ASCII Raster files may also be created by GIS applications, such as ArcMap or QGIS

Format

The first six lines contain metadata of the grid. Each line contains a label and a value. These lines are followed by a matrix with values listed in the order they would naturally appear (left-right, top-down). A PRJ[3] file is required for geo-referencing. For details, see
https://www.loc.gov/preservation/digital/formats/fdd/fdd000421.shtml

```
ncols       xxx
nrows       xxx
xllcorner   xxx
yllcorner   xxx
cellsize    xxx
NODATA_value  xxx
ZM1 ZM2 ZM3 ... ZMn
...
Z31 Z32 Z33 ... Z3n
Z21 Z22 Z23 ... Z2n
Z11 Z12 Z13 ... Z1n
```

Description

1. **ncols** and **nrows** are the numbers of columns and rows, respectively.

2. **xllcorner** and **yllcorner** are, respectively, the western (left) x-coordinate and southern (bottom) y-coordinate of the lower-left corner of the grid. Instead of xllcorner and yllcorner, xllcenter and yllcenter may be used. **xllcenter** and **yllcenter** are, respectively, the x and y coordinates of the center of the lower-left cell of the grid.

3. **cellsize** is the length of one side of a square cell. Instead of "cellsize xxx", a line with "DX xxx" and a line with "DY xxx" may be used. DX and DY are, respectively, the column and row widths of the raster.

4. **NODATA_value** is the value that is regarded as "missing" or "not applicable".

5. **The remainder of the file lists the raster values** for each cell, starting at the upperleft corner. These values are delimited using a single space character.

Example

The following is an example showing an ASCII Raster file for a grid with 4 columns and 3 rows.

```
NCOLS 4
NROWS 3
XLLCORNER -117.73
YLLCORNER 33.451
DX 400
```

```
DY 350
NODATA_value -1E20
11  12  34  23
42  35  23  21
23  41  31  19
```

5.1.6. Shapefile

The shapefile format is a binary format that is described in detail in ESRI white paper (ESRI, 1998).

5.1.7. MODPATH Starting Points

A MODPATH Starting Points file is a text file with the following format and can be exported or imported via MODPATH instances. See Section 4.2.4 for details about MODPATH instances.

File Format
1. #STARTINGLOCATION
2. Version
3. N

   (the following record repeats N times)
4. Layer, row, column, localX, localY, localZ, simulationTime

Description

- **#STARTINGLOCATION:** The first line holds the text string "#STARTINGLOCATION" that serves as the file format identifier.

- **Version** is reserved for file version. The default value of 1.0 should be used.

- **N** is the number of starting points (particles) saved in this file.

- **Layer, row, column, localX, localY, localZ, simulationTime:** each line represents a starting point.

    o **Layer, row,** and **column** are the cell where the particle is located.
    o **localX, localY,** and **localZ** are the local coordinates of the particle within the cell. The value of local coordinates range between 0 and 1.
    o **simulationTime** is the simulation time at which the particle is released.

5.1.8. Georeference file

A Georeference file is a text file with the following format. The file can be created by or loaded to the Georeference dialog box (see Figure 22 on page 35).

File Format
1. #GEOREFERENCE
2. Version
3. Method

4. Azimuth, Lat1, Lng1
5. LatUL, LngUL
6. LatUR, LngUR
7. LatLL, LngLL
8. LatLR, LngLR

Description

- **#GEOREFERENCE:** The first line holds the text string "#GEOREFERENCE" that serves as the file format identifier.

- **Version** is reserved for file version. The default value of 1.0 should be used.

- **METHOD** is the georeferencing method. Either 1 or 2 should be entered. If Method = 1, grid azimuth and coordinates of the lower-left grid corner, are used. If Method = 2, the coordinates of the four model grid corners are used to place the model grid on the map.

- **Azimuth, Lat1, Lng1:** These values are always read, but will be used only if Method = 1.

  - Azimuth is the angle in degrees measured clockwise from a meridian to the axis along the model's row direction. Enter 90 if the grid is not rotated.
  - Lat1 and Lng1: WGS-84 Latitude and longitude coordinates of the lower-left grid corner (i.e., outer corner of cell [NROW, 1]).

- **LatUL, LngUL, LatUR, LngUR, LatLL, LngLL, LatLR, LngLR:** These values are, respectively, the WGS-84 Latitude and longitude coordinates of the upper-left (cell[1,1]), upper-right (cell[1, NCOL]), lower-left (cell[NROW, 1]), and lower-right (cell[NROW, NCOL]) corners of model grid. These values are always read, but will be used only if Method = 2.

5.1.9. Observation File

Observation files are saved in the Microsoft Excel format. An observation file contains four sheets in the order of ObservationPoints, Head, Drawdown, and Concentration. See Section 3.5.3 for how to create or import an observation file.

1. **ObservationPoints:** The first row of this sheet contains the column headers **Active, PointName, Label, Layer, Latitude,** and **Longitude.** The remaining rows contains the data of the observation points.

   - **Active** is either 1 (the observation point is active) or 0 (the observation point is inactive).

   - **PointName** is the unique name of the observation point.

   - **Label** will be displayed next to the observation point on the map. Use "\n" to move to next line; "\u" to move to previous line; and "\\" for backslash. Only ASCII characters with ASCII values from 32 to 126 are supported.

   - **Layer** is the model layer, to which the observation point belongs.

- **Latitude** and **Longitude** are the coordinates of the observation point in the WGS-84 datum.

2. **Head** and **Drawdown:** The first row of this sheet contains the column headers **PointName, SimulationTime, Value, Weight,** and **DateTime.** The remaining rows contains the data of the head or drawdown observations.

   - **PointName** is the name of the observation point, at which the observations are made.

   - **Value** is the observed value.

   - **SimulationTime** is the observation time, expressed in the simulation time. If you prefer to use calendar date/time, leave this cell blank.

   - **Weight**: The Weight of an observation gives a relative confidence level of the observed value. The higher the Weight value, the better is the measurement. The weight can be set at zero if needed (meaning that the observation takes no part in the calculation of the objective function during a parameter estimation process), but it must not be negative. Refer to the PEST User Manual (Doherty, 2016) for the function of weights in the parameter estimation process.

   - **DateTime** is the observation calendar date/time, for example 12/31/2019 23:59:59[50]. This value is used only if the SimulationTime cell is blank. During the import process, PM determines the corresponding SimulationTime based on the model start date/time and the given DateTime.

3. **Concentration:** The first row of this sheet contains the column headers **PointName, SimulationTime, Value, Weight,** and **Species.** The remaining rows contains the data of the concentration observations.

   - **PointName, Value, SimulationTime, Weight,** and **DateTime:** These are the same as the respective values described above for Head and Drawdown.

   - **Species:** Name of the species that is one of the Species Names defined in the Species tab of the Transport Settings dialog box (see Section 3.8.3.1).

5.1.10. Polygon File

A Polygon file is a text file with the following format. You can export or import polygon files via the Data Editor, see Section 3.3.2.3 for details.

Format
1. #PM_POLYGONS
2. Version
3. NPolygons

(repeat the following data block, i.e., data 4 – 13, NPolygons times; a block for a polygon)

---

[50] If the time portion is omitted, the time is assumed to be 00:00:00. Note that Excel internally stores the calendar date/time as a floating value. The displayed date/time string may be different based on your locale and/or format settings.

4. DataVersion

5. Name

6. IsOn, IsHole, AutoLayerNumber, ShowVertices, Priority

7. LineWidth, Red, Green, Blue

8. NP

9. Longitude, Latitude (repeat NP times)

10. NValues

11. Value (an array of NValues values separated by space or in different lines)

12. NVars

13. Var (an array of NVars values separated by space or in different lines)

14. NConcs

15. Conc (an array of NConcs values separated by space or in different lines)

Description

- **#PM_POLYGONS:** The first line holds the text string "#PM_POLYGONS" that serves as the file format identifier.

- **Version** is the version number that is reserved for future use. The value for the current version is 1.

- **NPolygons** is the number of polygons.

- **DataVersion** is the version number of the data block. The value for the current DataVersion is 1.01

- **Name** is the name of the polygon

- **IsOn** is a value equals to either 1 or 0. The value of 1 means that the polygon is turned on; 0 means off.

- **IsHole** is a value equals to either 1 or 0. The value of 1 means that the polygon represents a hole; 0 means not a hole.

- **AutoLayerNumber** is a value equals to either 1 or 0. The value of 1 means that when applying the polygon to cells, the auto layer number feature is on; 0 means off.

- **ShowVertices** is a value equals to either 1 or 0. The value of 1 means that the vertices of the polygon is displayed; 0 means not displayed.

- **Priority:** When applying overlapping polygons to cells, the polygon with the smallest priority value has the highest priority.

- **LineWidth:** This value is reserved for future use. It should be 2.

- **Red, Blue, Green:** These values are reserved for future use. They should range between 0 and 255.

- **NP:** Number of vertices of the polygon. A polygon must have at least 6 vertices. The number of vertices must be even. The odd numbered vertices are big white vertices (see Section 3.3.2.3 for the vertex types), the even numbered vertices are small grey vertices.

- **Longitude, Latitude** are coordinates of the vertex expressed in the WGS 84 geographical coordinates.

- **NValues** and **Value**: **Value** is an array of values that are assigned to the polygon and **NValues** is the size of the Value array. The Value array may contain values of -999999999, which indicates a NotDefinedValue. As given below, the size and contents of the Value array vary with the parameter/package that is being edited. Refer to Section 3.8.1.1 for details about package-specific data.

  o For Layer Top Elevation, Layer Bottom Elevation, IBOUND, ICBUND, Starting Hydraulic Head, Effective Porosity, Retardation Factor, Bulk Density, Sand Box 1, Sand Box 2, Sand Box 3, Wetting Threshold, and all data of the ZoneBudget and MT3D/SEAWAT menus: NValues = 1 and Value[1] contains the respective value of these properties.

  o For aquifer properties, such as Horizontal Hydraulic Conductivity, Vertical Hydraulic Conductivity, Specific Storage, Horizontal Anisotropy, Vertical Anisotropy, Transmissivity, Vertical Leakance, Storage Coefficient, and Specific Yield: NValues = 2.

    – Value[1] = the respective aquifer property value.
    – Value[2] = Parameter Number [-].

  o **CHD:** NValues = 5.

    – Value[1] = Flag [-].
    – Value[2] = Start Head (h_s) [L].
    – Value[3] = End Head (h_e) [L].
    – Value[4] = Head Conversion [-] (SEAWAT) [-].
    – Value[5] = Water Density (d) [ML^{-3}] (SEAWAT).

  o **DRN:** NValues = 4.

    – Value[1] = Drain conductance (C_d) per unit area [T^{-1}].
    – Value[2] = Drain elevation (h_d) [L].
    – Value[3] = Parameter Number [-].
    – Value[4] = Elevation of drain bottom [L].

  o **DRT1:** NValues = 8.

    – Value[1] = Drain conductance (C_d) per unit area [T^{-1}].
    – Value[2] = Drain elevation (h_d) [L].
    – Value[3] = Column number of the return flow recipient cell [-].
    – Value[4] = Row number of the return flow recipient cell [-].

- Value[5] = Layer number of the return flow recipient cell [-].
- Value[6] = Return flow proportion [-].
- Value[7] = Parameter Number [-].
- Value[8] = Elevation of drain bottom [L].
- Value[9] = Return flow On/Off [-]. 1= on; 0 =off.

o **ETS1:** NValues = 5 + 2 x (NS – 1), where NS is the number of segments.

- Value[1] = Maximum ET Flux (ETSR) [LT^{-1}].
- Value[2] = Elevation of ET Surface (ETSS) [L].
- Value[3] = ET Extinction Depth (ETSX) [L].
- Value[4] = Layer Indicator (IETS) [-].
- Value[5] = Parameter Number [-].
- Value[5 + i] = PXDP [-] of the i-th segment.
- Value[5 + i * 2] = PETM [-] of the i-th segment.

o **EVT**: NValues = 5

- Value[1] = Maximum ET Flux (EVTR) [LT^{-1}].
- Value[2] = Elevation of ET Surface (SURF) [L].
- Value[3] = ET Extinction Depth (ETDP) [L].
- Value[4] = Layer Indicator (IEVT) [-].
- Value[5] = Parameter Number [-].

o **FHB1**: NValues = 2

- Value[1] = boundary type

  - 0: none
  - 1: specified head
  - 2: specified flow

- Value[2] = Cell Face (IAUX)

  - 0: Internal distributed source/sink
  - 1: Left
  - 2: Right
  - 3: Front
  - 4: Rear
  - 5: Bottom
  - 6: Top
  - 7: Lateral Faces

o **GHB**: NValues = 5

- Value [1] = Boundary conductance per unit area [T^{-1}].
- Value [2] = Hydraulic Head on External Source (HB) [L].

- Value[3] = GHB Elevation (SEAWAT) [L].
- Value[4] = Water Density at GHB (SEAWAT) [L].
- Value[5] = Parameter Number [-].

- **IBS:** NValues = 5

  - Value[1] = Preconsolidation Head (HC) [L].
  - Value[2] = Elastic Storage Factor (Sfe) [-].
  - Value[3] = Inelastic Storage Factor (Sfv) [-].
  - Value[4] = Starting Compaction (COM) [L].
  - Value[5] = Parameter Number [-].

- **RCH:** NValues = 3

  - Value[1] = Recharge Flux (RECH) [LT^{-1}].
  - Value[2] = Layer Indicator (IRCH) [-].
  - Value[3] = Parameter Number [-].

- **RES1**: NValues = 6

  - Value[1] = Reservoir Number (IRES) [-].
  - Value[2] = Land Surface Elevation (Bres) [L].
  - Value[3] = Vertical Hydraulic Conductivity (HCres) [LT^{-1}].
  - Value[4] = Reservoir Bed Thickness (Rbthck) [L].
  - Value[5] = Layer Number (IRESL) [-].
  - Value[6] = Parameter Number [-].

- **RIV**: NValues = 6

  - Value[1] = Riverbed conductance per unit area C_{riva} [T^{-1}].
  - Value[2] = River Stage h_{riv} [L].
  - Value[3] = Elevation of the Riverbed Bottom (B_{riv}) [L].
  - Value[4] = Thickness of Riverbed Sediments (SEAWAT) [L].
  - Value[5] = River Water Density (SEAWAT) [ML^{-3}].
  - Value[6] = Parameter Number [-].

o **SWI2:** NValues = 10.

  - Value[1] = ISOURCE.
  - Value[2] = Initial elevation of Zeta surface 1 [L].
  - Value[3] = Initial elevation of Zeta surface 2 [L].
  - Value[4] = Initial elevation of Zeta surface 3 [L].
  - Value[5] = Initial elevation of Zeta surface 4 [L].
  - Value[6] = Initial elevation of Zeta surface 5 [L].
  - Value[7] = Initial elevation of Zeta surface 6 [L].
  - Value[8] = Initial elevation of Zeta surface 7 [L].

- Value[9] = Initial elevation of Zeta surface 8 [L].
- Value[10] = Initial elevation of Zeta surface 9 [L].

o **UZF1:** NValues = 11.

- Value[1] = Aerial Extent (IUZFBND).
- Value[2] = Vertical Saturated Hydraulic Conductivity (VKS) [LT^{-1}].
- Value[3] = Brooks-Corey Epsilon (EPS) [-].
- Value[4] = Saturated Water Content (THTS) [L^3L^{-3}].
- Value[5] = Residual Water Content (THTR) [L^3L^{-3}].
- Value[6] = Initial Water Content (THTI) [L^3L^{-3}].
- Value[7] = Infiltration Rate (FINF) [LT^{-1}].
- Value[8] = Potential ET (PET) [LT^{-1}].
- Value[9] = ET Extinction Depth (EXTDP) [L].
- Value[10] = ET Extinction Water Content (EXTWC) [L^3L^{-3}].
- Value[11] = Parameter Number [-].

o **WEL:** NValues = 3.

- Value[1] = Flow Rate per unit area [LT^{-1}]:
- Value[2] = Fluid Density (SEAWAT) [ML^{-3}].
- Value[3] = Parameter Number [-].

- **NVars** and **Var** are used to define the time series of prescribed flux or head in the FHB1 package. **Var** is the time series array and **NVars** is the size of array.

- **NConcs** and **Conc** are used to define the concentration values associated with species. **Conc** an array containing concentration data of individual species and **NConcs** is the size of the Conc array. NConcs is limited to a maximum of 100.

5.1.11. Polyline File

A Polyline file is a text file with the following format. You can export or import polyline files via the Data Editor, see Section 3.3.2.2 for details.

Format
1. #PM_POLYLINES
2. Version
3. NPolylines

(repeat the following data block, i.e., data 4 – 15, NPolylines times; a block for a polyline)

4. DataVersion
5. Name
6. IsOn, AutoLayerNumber, ShowVertices, Priority
7. LineWidth, Red, Green, Blue
8. NProperties

9. Property (an array of NProperties values separated by space)

10. NP

(repeat the following data block NP times; a block for a vertex)

11. VertexDataVersion

12. Vertex_id

13. Att1

14. Longitude, Latitude

15. NValues

16. Value (an array of NValues values separated by space or in different lines)

17. NVars

18. Var (an array of NVars values separated by space or in different lines)

19. NConcs

20. Conc (an array of NConcs values separated by space or in different lines)

21. Naux1

22. Aux1 (an array of Naux1 values separated by space or in different lines)

23. Naux2

24. Aux2 (an array of Naux2 values separated by space or in different lines)

Description

- **#PM_POLYLINES:** The first line holds the text string "#PM_POLYLINES" that serves as the file format identifier.

- **Version** is the version number that is reserved for future use. The value for the current version is 1.04

- **NPolylines** is the number of polylines.

- **DataVersion** is the version number of the data block. The value for the current DataVersion is 1.

- **Name** is the name of the polyline.

- **IsOn** is a value equals to either 1 or 0. The value of 1 means that the polyline is turned on; 0 means off.

- **AutoLayerNumber** is a value equals to either 1 or 0. The value of 1 means that when applying the polyline to cells, the auto layer number feature is on; 0 means off.

- **ShowVertices** is a value equals to either 1 or 0. The value of 1 means that the vertices of the polyline is displayed; 0 means not displayed.

- **Priority:** When applying overlapping polyline to cells, the polyline with the smallest priority value has the highest priority.

- **LineWidth:** This value is reserved for future use. It should be 2.

- **Red, Blue, Green:** These values are reserved for future use. They should range between 0 and 255.

- **NProperties** and **Properties. NProperties** is number of polyline properties. **Properties** is the array of polyline properties. Polyline properties are used by the following packages. For all other packages or aquifer properties, NProperties should be set to zero.

    o **CHD**: NProperties = 1

        – Property[1] defines Head Conversion Option for SEAWAT as follows

            ▪ 0: Use calculated water density at the cell
            ▪ 1: Use the specified water density value
            ▪ 2: Use the average of the calculated water density of the overlying cells
            ▪ 3: Input head values are reference head. No conversion

    o **DRT**: NProperties = 1

        – Property[1] controls whether Return flow is On or Off.

            ▪ 0: Return flow is off.
            ▪ 1: Return flow is on.

    o **FHB:** NProperties = 2

        – Property[1] is the boundary type

            ▪ 0: none
            ▪ 1: specified head
            ▪ 2: specified flow

        – Property[2] defines the Cell Face (IAUX)

            ▪ 0: Internal distributed source/sink
            ▪ 1: Left
            ▪ 2: Right
            ▪ 3: Front
            ▪ 4: Rear
            ▪ 5: Bottom
            ▪ 6: Top
            ▪ 7: Lateral Faces

    o **SFR2**: NProperties = 1

            ▪ Property[1] is the Segment Number

    o **STR**: NProperties = 2

        – Property[1] is the Segment Number
        – Property[2] is the Segment Inflow.

- **NP:** Number of vertices of the polyline. A polyline must have at least 3 vertices. The number of vertices must be odd. The odd numbered vertices are big white vertices (see Section 3.3.2.3 for the vertex types), the even numbered vertices are small grey vertices.

- **VertexDataVersion** is the version number of the vertex block. The value for the current VertexDataVersion is 1.01.

- **Vertex_id,** introduced since VertexDataVersion 1.01, is the unique identifier of the vertex.

- **Att1,** introduced since VertexDataVersion 1.04, is an attribute of the vertex.

- **Longitude, Latitude** are coordinates of the vertex expressed in the WGS 84 geographical coordinates.

- **NValues** and **Value**: **Value** is an array of values that are assigned to the vertex. NValues is the size of the Value array. Note that a Value array may only be assigned to odd numbered vertices. Values that are assigned to even numbered vertices will be discarded. The Value array may contain values of -999999999, which indicates a NotDefinedValue. As given below, the size and contents of the Value array vary with the parameter/package that is being edited. Refer to Section 3.8.1.1 for details about package-specific data.

  o For Layer Top Elevation, Layer Bottom Elevation, IBOUND, ICBUND, Starting Hydraulic Head, Effective Porosity, Retardation Factor, Bulk Density, Sand Box 1, Sand Box 2, Sand Box 3, Wetting Threshold, and all data of the ZoneBudget and MT3D/SEAWAT menus: NValues = 1 and Value[1] contains the respective value of these properties.

  o For aquifer properties, such as Horizontal Hydraulic Conductivity, Vertical Hydraulic Conductivity, Specific Storage, Horizontal Anisotropy, Vertical Anisotropy, Transmissivity, Vertical Leakance, Storage Coefficient, and Specific Yield: NValues = 2.

    – Value[1] = the respective aquifer property value.
    – Value[2] = Parameter Number [-].

  o **DRN:** NValues = 4.

    – Value[1] = Drain conductance per unit length [LT^{-1}].
    – Value[2] = Drain elevation (h_d) [L].
    – Value[3] = Parameter Number [-].
    – Value[4] = Elevation of drain bottom [L].

  o **DRT1:** NValues = 8.

    – Value[1] = Drain conductance per unit length [LT^{-1}].
    – Value[2] = Drain elevation (h_d) [L].
    – Value[3] = Column number of the return flow recipient cell [-].
    – Value[4] = Row number of the return flow recipient cell [-].
    – Value[5] = Layer number of the return flow recipient cell [-].

- Value[6] = Return flow proportion [-].
- Value[7] = Parameter Number [-].
- Value[8] = Elevation of drain bottom [L].

o **ETS1:** NValues = 5 + 2 x (NS – 1), where NS is the number of segments.

- Value[1] = Maximum ET Flux (ETSR) [LT^{-1}].
- Value[2] = Elevation of ET Surface (ETSS) [L].
- Value[3] = ET Extinction Depth (ETSX) [L].
- Value[4] = Layer Indicator (IETS) [-].
- Value[5] = Parameter Number [-].
- Value[5 + i] = PXDP [-] of the i-th segment.
- Value[5 + i * 2] = PETM [-] of the i-th segment.

o **EVT**: NValues = 5

- Value[1] = Maximum ET Flux (EVTR) [LT^{-1}].
- Value[2] = Elevation of ET Surface (SURF) [L].
- Value[3] = ET Extinction Depth (ETDP) [L].
- Value[4] = Layer Indicator (IEVT) [-].
- Value[5] = Parameter Number [-].

o **FHB1**: NValues = 0

o **GHB**: NValues = 5

- Value[1] = Boundary conductance per unit length [LT^{-1}].
- Value[2] = Hydraulic Head on External Source (HB) [L].
- Value[3] = GHB Elevation (SEAWAT) [L].
- Value[4] = Water Density at GHB (SEAWAT) [L].
- Value[5] = Parameter Number [-].

- **IBS:** NValues = 5

- Value[1] = Preconsolidation Head (HC) [L].
- Value[2] = Elastic Storage Factor (Sfe) [-].
- Value[3] = Inelastic Storage Factor (Sfv) [-].
- Value[4] = Starting Compaction (COM) [L].
- Value[5] = Parameter Number [-].

- **RCH:** NValues = 3

- Value[1] = Recharge Flux (RECH) [LT^{-1}].
- Value[2] = Layer Indicator (IRCH) [-].
- Value[3] = Parameter Number [-].

- **RIV**: NValues = 6

- Value[1] = Riverbed conductance per unit length C_{rivl} [LT^{-1}].
- Value[2] = River Stage h_{riv} [L].
- Value[3] = Elevation of the Riverbed Bottom (B_{riv}) [L].
- Value[4] = Thickness of Riverbed Sediments (SEAWAT) [L].
- Value[5] = River Water Density (SEAWAT) [ML^{-3}].
- Value[6] = Parameter Number [-].

- **SFR2**: NValues = 16.

  - Value[1] = Stream slope (SLOPE) [-].
  - Value[2] = Top Elevation of the Streambed (STRTOP) [L]:
  - Value[3] = Thickness of the Streambed (STRTHICK) [L].
  - Value[4] = Streambed Hydraulic Conductivity (STRHC1) [LT^{-1}].
  - Value[5] = Saturated Volumetric Water Content (THTS) [-].
  - Value[6] = Initial Volumetric Water Content (THTI) [-]:
  - Value[7] = Brooks-Corey Exponent (EPS) [-].
  - Value[8] = Vertical Saturated Hydraulic Conductivity (UHC) [LT^{-1}].
  - Value[9] = Parameter Number (PEST) [-].
  - Value[10] – Value[16]: reserved and not used.

- **STR**: NValues = 8. Assign -999999999 to Value[5], Value[6], and Value[7], if *Stream Stage in Reaches* is not to be calculated.

  - Value[1] = Stream Stage (h_{str}) [L].
  - Value[2] = Streambed Conductance (C_{str}) [L^{2}T^{-1}].
  - Value[3] = Elevation of Streambed Top (T_{str}) [L].
  - Value[4] = Elevation of Streambed Bottom (B_{str}) [L].
  - Value[5] = Width of the Stream Channel (W_{str}) [L].
  - Value[6] = Slope of the Stream Channel (S_{str}) [-].
  - Value[7] = Manning's Roughness Coefficient (n) [TL$^{-1/3}$].
  - Value[8] = Parameter Number [-].

o **SWI2:** NValues = 10.

  - Value[1] = ISOURCE.
  - Value[2] = Initial elevation of Zeta surface 1 [L].
  - Value[3] = Initial elevation of Zeta surface 2 [L].
  - Value[4] = Initial elevation of Zeta surface 3 [L].
  - Value[5] = Initial elevation of Zeta surface 4 [L].
  - Value[6] = Initial elevation of Zeta surface 5 [L].
  - Value[7] = Initial elevation of Zeta surface 6 [L].
  - Value[8] = Initial elevation of Zeta surface 7 [L].
  - Value[9] = Initial elevation of Zeta surface 8 [L].
  - Value[10] = Initial elevation of Zeta surface 9 [L].

- o **UZF1:** NValues = 11.

  - Value[1] = Aerial Extent (IUZFBND).
  - Value[2] = Vertical Saturated Hydraulic Conductivity (VKS) $[LT^{-1}]$.
  - Value[3] = Brooks-Corey Epsilon (EPS) [-].
  - Value[4] = Saturated Water Content (THTS) $[L^3L^{-3}]$.
  - Value[5] = Residual Water Content (THTR) $[L^3L^{-3}]$.
  - Value[6] = Initial Water Content (THTI) $[L^3L^{-3}]$.
  - Value[7] = Infiltration Rate (FINF) $[LT^{-1}]$.
  - Value[8] = Potential ET (PET) $[LT^{-1}]$.
  - Value[9] = ET Extinction Depth (EXTDP) [L].
  - Value[10] = ET Extinction Water Content (EXTWC) $[L^3L^{-3}]$.
  - Value[11] = Parameter Number [-].

- o **WEL:** NValues = 3.

  - Value[1] = Flow Rate per unit length $[L^2T^{-1}]$:
  - Value[2] = Fluid Density (SEAWAT) $[ML^{-3}]$.
  - Value[3] = Parameter Number [-].

- **NVars** and **Var** are used to define the time series of prescribed flux or head in the FHB1 package. **Var** is the time series array and **NVars** is the size of array.

- **NConcs** and **Conc** are used to define the concentration values associated with species. **Conc** an array containing concentration data of individual species and **NConcs** is the size of the Conc array. NConcs is limited to a maximum of 100.

- **Naux1** and **Aux1** are introduced in VertexDataVersion 1.04 and are currently only used by SFR2 package to define the initial concentration values associated with species. Those values are intended to be used by the SFT Package. **Aux1** an array containing concentration data of individual species and **Naux1** is the size of the **Aux1** array. **Naux1** is limited to a maximum of 100.

- **Naux2** and **Aux2** are introduced in VertexDataVersion 1.04 and are currently only used by SFR2 package to define the stream dispersion values associated with species. Those values are intended to be used by the SFT Package. **Aux2** an array containing concentration data of individual species and **Naux2** is the size of the **Aux2** array. **Naux2** is limited to a maximum of 100.

5.1.12. Reservoir Stage Time Series

A Reservoir Stage Time Series file is a text file that contains the stage measurements of reservoirs that are used by the Reservoir Package (RES1). You can export or import reservoir stage time series files via the Reservoir Stage Time Series dialog box (Figure 66).

Format

1. #RESERVOIR_STAGE_SERIES

2. Version

3. NRES

   (repeat the following block NRES times)

4. ReserviorNumber, ReservoirName

5. N

   (repeat the following line N times)

6. Time, Stage

Description

- **#RESERVOIR_STAGE_SERIES:** The first line holds the text string "#RESERVOIR_STAGE_SERIES" that serves as the file format identifier.

- **Version** is the version number that is reserved for future use. The value for the current version is 1.

- **NRES** is the number of reservoirs.

- **ReserviorNumber** and **ReservoirName** are the number and name of the reservoir, respectively.

- **N** is the number of data points that will follow.

- **Time** and **Stage** are the simulation time and the reservoir stage, respectively.

5.1.13. Series File

A Series file is a text file that contains a series of numbers. Many dialog boxes of PM can load or save Series files.

Format

1. #SERIES

2. Version

3. N

4. v(1) v(2) v3 …. v(N)

Description

- **#SERIES:** The first line holds the text string "#SERIES" that serves as the file format identifier.

- **Version** is the version number that is reserved for future use. The value for the current version is 1.

- **N** is the number of values that will follow.

- **v(1), v(2), …, v(N)** are the values of the series. These values must be separated by a space or comma, or in different lines.

5.1.14. SURFER ASCII GRD File

A SURFER GRD file may only be imported to regularly spaced model grids. PM only accepts SURFER ASCII GRD files. Binary GRD files cannot be imported.

Format

    DSAA
    ncols nrows
    Xmin Xmax
    Ymin Ymax
    Zmin Zmax
    Z11 Z12 Z13 ... Z1n
    Z21 Z22 Z23 ... Z2n
    Z31 Z32 Z33 ... Z3n
    ...
    ZM1 ZM2 ZM3 ... ZMn

Description

1. **DSAA**: The first line holds the ASCII (text) string "DSAA" that serves as the file format identifier.

1. **ncols** and **nrows** are the numbers of columns and rows, respectively.

2. **Xmin Xmax** are the minimum and maximum x values, respectively.

3. **Ymin Ymax** are the minimum and maximum y values, respectively.

4. **Zmin Zmax** are the minimum and maximum z values, respectively.

5. **The remainder of the file lists the matrix values**, starting at the lower-left corner (i.e., Z11). These numbers are delimited using a single space character. Note that the first row is the one associated with the minimum value of y and represents the bottom edge of your map. The last row is the top edge of the map. The leftmost value in each row is that associated with the minimum x, the rightmost goes with the maximum x.

Example

The following is an example showing an ASCII Raster file for a grid with 4 columns and 3 rows.

    DSAA
    4 3
    -117.73 -117.71
    33.451 33.471
    11 42
    23 41 31 19
    42 35 23 21
    11 12 34 23

5.1.15. Temporal Discretization File

A temporal discretization file is a text file that contains the temporal discretization data that can be exported from or imported to the Time dialog box (see Section 3.6.1).

File Format
1. #TemporalDiscretization
2. Version
3. NPER TimeUnit

   (the following line repeats NPER times)
4. IsSteady, PERLEN, NSTP, TSMULT, DT0, MXSTRN, TTSMULT, TTSMAX, FLAG

Description
- **#TemporalDiscretization:** The first line holds the text string "#TemporalDiscretization" that serves as the file format identifier.

- **Version** is the version number that is reserved for future use. The value for the current version is 1.

- **NPER** is the number of stress periods

- **TimeUnit** is an integer between 0 and 4: 0 = Second; 1 = Minute; 2 = Hour; 3 = Day; 4 = Year.

- **IsSteady** > 0 if the stress period is steady state. **IsSteady** = 0 for a transient stress period.

- **PERLEN** is the length of the stress period, in the unit of TimeUnit.

- **NSTP** is the number of time steps within a stress period.

- **TSMULT** is the time step multiplier, which is the ratio of the length of each time step to that of the preceding time step.

- **DT0** is the initial transport step length within each time step of the flow solution.

- **MXSTRN** is the maximum number of transport steps allowed within one time step of the flow solution.

- **TTSMULT** is the multiplier for successive transport steps within a flow time step.

- **TTSMAX** is the maximum transport step size.

- **FLAG** is an integer reserved for future use. It should be set as zero.

5.1.16. Well File

A Well File contains the meta data of wells (name, location, and screen intervals) and the pumping time series as given below. A Well File is not the same as the input file to the Well Package that is defined in the user guide of MODFLOW-2005 (Harbaugh, 2005). Well files may be imported to the Well Package. See Sections 3.5.20 and 3.8.1.1.20 for details.

File Format

1. #WellFile

   (repeat the following line for each well)

2. WellName, Latitude, Longitude, Top1, Bottom1, [Top2, Bottom2]…

3. #Pumping

   (repeat the following line for the periods at which pumping/injection are to be assigned)

4. p, Q_w1_p, Q_w2_p, …, Q_wn_p

   The following data are optional and are needed only if you need to assign concentration values to inject wells.

5. [#Concentration]

   (repeat the following optional line for the periods at which the concentration values of the corresponding injection are to be assigned)

6. [p, C_w1_p, C _w2_p, …, C_wn_p]

Description

- **#WellFile:** The first line holds the text string "#WellFile" that serves as the file format identifier.

- **Wellname** is well name. Wellname may contain spaces but may not include comma.

- **Latitude** and **Longitude** are the coordinates of the well in the WGS-84 datum.

- **Top1** and **Bottom1** are the top and bottom elevation of the first screen interval. Repeat the elevation pairs from top down as needed.

- **#Pumping.** The line starting with "#Pumping" (or "#Period") is used to terminate the well information and to denote the start of the pumping data.

- **p** is the period number at which the pumping/injection rates or concentration values are to be assigned.

- **Q_w1_p, Q_w2_p, …, Q_wn_p** are the pumping/injection rate of well 1, well 2, …, well n in the period **p**. These values must be given in the same order as the wells appear in Data 2. Use negative values for pumping; positive values for injection.

- **#Concentration.** The line starting with "#Concentration" is used to terminate the pumping data and to denote the start of the concentration data. This line is optional.

- **C_w1_p, C_w2_p, …, CQ_wn_p** are the concentration values of well 1, well 2, …, well n in the period **p**. This line is optional. The values must be given in the same order as the wells appear in Data 2. Concentration values must be greater or equal to zero and are only effective at injection wells. Negative concentration values and concentration values that are assigned to pumping wells are ignored.

Example

Table 5 shows the coordinates, screen interval, and pumping/injection rates of three wells. For Well 3, the concentration values of the injection are 100 and 200 for period 1 and 2, respectively. The corresponding Well File for these wells is as follows.

```
#WellFile
Well 1, 34.12, -117.33, 100, 90, 60, 40
Well 2, 34.56, -117.67, 80, 50
Well 3, 34.22, -117.28, 82, 43
#Pumping
1, -50, -45, 25
2, -60, -55, 40
#Concentration
1, 0, 0, 100
2, 0, 0, 200
```

Table 5. Well Data Example

Well Name	Latitude	Longitude	Top1	Bottm1	Top2	Bottom2	Pumping (period 1)	Pumping (period 2)
Well 1	34.12	-117.33	100	90	60	40	-50	-60
Well 2	34.56	-117.67	80	50			-45	-55
Well 3	34.22	-117.28	82	43			25	40

5.2. Input and Output Data Files of the Supported Models

This section lists the names of the input and output files of the supported model codes and packages. Refer to the documents of the model codes for details about the file formats. By default, all input and output files of a model are stored in the *model data folder*. The name of this folder is ModelID and it can be found in the same folder as the PM file. In addition to the input and output files given in this section, PM will create and maintain several binary files in the "binary" subfolder of the model data folder. These binary files are used by PM to display cell information on the Properties window.

5.2.1. MODFLOW-2005/MODFLOW-NWT

5.2.1.1. Input Files

Basic Package	modflow.bas6
Block-Centered Flow Package	modflow.bcf6
Discretization	modflow.dis
Direct Solver Package	modflow.de4
Drain Package	modflow.drn
Drain with Return Flow Package	modflow.drt
Evapotranspiration Package	modflow.evt

Evapotranspiration Segments Package	modflow.ets
Flow and Head Boundary Package	modflow.fhb
General-Head Boundary Package	modflow.ghb
Generic Multigrid Solver Package	modflow.gmg
Horizontal-Flow Barrier Package	modflow.hfb6
Interbed-Storage Package	modflow.ibs
Lake Package	modflow.lak
Layer-Property Flow Package	modflow.lpf
LMT Package	modflow.lmt
Multi-Node Well 1 Package	modflow.mnw1
Newton Solver Package	modflow.nwt
Name File	modflow.nam
Output Control	modflow.oc
Preconditioned Conjugate Gradient (PCG) Solver Package	modflow.pcg
PCG Solver with Improved Nonlinear Control Package	modflow.pcgn
Recharge Package	modflow.rch
Reservoir Package	modflow.res1
River Package	modflow.riv
Seawater Intrusion 2 Package	modflow.sw
Stream (STR) Package	modflow.str
Streamflow-Routing (SFR2) Package	modflow.sfr
Strongly Implicit Procedure Solver Package	modflow.sip
Subsidence and Aquifer-System Compaction Package	mudflow.sub
Time Variant Specified Head	modflow.chd
Unsaturated-Flow Package	modflow.uzf
Upstream Weighting Package	modflow.upw
Well Package	modflow.wel

5.2.1.2. Output Files

Run Listing	modflow.list
Drawdown	modflow.drawdown
Flow (cell-by-cell flow terms)	modflow.flow
Flow-transport link	modflow.linkmt3d
Hydraulic head	modflow.head
Interbed-Storage Package	modflow.interbed
Seawater Intrusion 2 Package	modflow.swi2zeta
Streamflow-Routing (SFR2) Package	modflow.sfr2.list
Subsidence and Aquifer-System Compaction Package[51]	modflow.subsidence, modflow.compaction, modflow.zdisplacement

---

[51] Output files are optional and defined in the Options tab of the Subsidence and Aquifer Compaction dialog box (Figure 76)

5.2.2. MT3DMS/MT3D-USGS

5.2.2.1.   Input Files

Advection Package	mt3d.adv
Basic Transport Package	mt3d.btn
Dispersion Package	mt3d.dsp
Flow-transport link[52]	modflow.linkmt3d
Generalized Conjugate Gradient Solver Package	mt3d.gcg
Lake Transport Package	mt3d.lkt
Name File	mt3d.nam
Reaction Package	mt3d.rct
Sink/Source Mixing Package	mt3d.ssm
Streamflow Transport Package	mt3d.sft

5.2.2.2.   Output Files

Run Listing	mt3d.list
Concentration for the dissolved-phase	MT3Dnnn.UCN[53]
Concentration for the sorbed-phase	MT3DnnnS.UCN[53]
Mass budget summary	MT3Dnnn.MAS[53]
Streamflow Transport Package Observation	mt3d.sft.obs

5.2.3. SEAWAT

This section lists the input files specific to SEAWAT. In addition to these files, all input and output files of MODFLOW and MT3D-USGS may be included in a SEAWAT simulation run.

5.2.3.1.   Input Files

Name File	seawat.nam
Variable Density Package	seawat.vdf
Viscosity Package	seawat.vsc

5.2.3.2.   Output Files

Listing File	seawat.list

5.2.4. MODPATH

Most input and output files of a MODPATH instance use *MODPATH-InstanceID* as their base filename. The *InstanceID* is a string consists of 5-characters displayed on the Settings window of the MODPATH instance.

5.2.4.1.   Input Files

Simulation	MODPATH-InstanceID.sim

---

[52] This file is created by a MODFLOW run.
[53] "nnn" is the species index number, such as 001 for species 1, 002 for species 2, and so on.

Basic Data	MODPATH-InstanceID.bas
Discretization	modflow.dis
Flow (cell-by-cell flow terms)[52]	modflow.flow
Hydraulic head[52]	modflow.head
Name File	MODPATH-InstanceID.nam
Starting Location	MODPATH-InstanceID.locations

5.2.4.2.   Output Files

Pathline	MODPATH-InstanceID.pathline
Endpoint	MODPATH-InstanceID.endpoint
Time Series	MODPATH-InstanceID.timeseries

5.2.5. PEST

5.2.5.1.   Input Files

Bore Coordinate	pest.borecoordinate
Control Data	pest.pst
Drawdown Instruction	pest.drawdowninstruction
Grid Specification	pest.gridspecification
Head Instruction	pest.headinstruction
Mod2SMP Input for extracting head results	pest.mod2smpheadinput
Mod2SMP Input for extracting drawdown results	pest.mod2smpdrawdowninput
Settings	settings.fig

Template Files

Block-Centered Flow Package	pest.bcf6
Drain Package	pest.drn
Drain with Return Flow Package	pest.drt
Evapotranspiration Package	pest.evt
Evapotranspiration Segments Package	pest.ets
General-Head Boundary Package	pest.ghb
Horizontal-Flow Barrier Package	pest.hfb6
Interbed-Storage Package	pest.ibs
Lake Package	pest.lak
Layer-Property Flow Package	pest.lpf
Recharge Package	pest.rch
Reservoir Package	pest.res1
River Package	pest.riv
Stream (STR) Package	pest.str
Unsaturated-Flow Package	pest.uzf
Upstream Weighting Package	pest.upw
Well Package	pest.wel

5.2.5.2.   Output Files

Run Record	pest.rec
Estimated Parameter Values	pest.par
Iteration Specific Parameter Values	pest.par.n[54]
Run Specific Parameter Value	pest.par.n_m[54]
Residuals	pest.res
Interim Residuals	pest.rei
Iteration Specific Residuals	pest.rei.n[54]
Composite Parameter Sensitivities	pest.sen
Composite Observation Sensitivities	pest.seo
SVD Output	pest.svd
Matrix	pest.mtt
Resolution Data	pest.rsd
Jacobian Matrix	pest.jco
Iteration Specific Jacobian Matrix	pest.jco.n[54]
Run Management Record	pest.rmr

5.2.5.3.   Batch Files for starting PEST or BeoPEST

PEST Batch File	pest.bat
PESTCHEK Batch File	pestchek.bat
Model Run Batch File	moderun.bat
BeoPEST Master Batch File	BeoPEST.bat[55]
BeoPEST Agent Batch File	BeoPEST_slave.bat[56]
BeoPEST Agents Batch File	BeoPEST_slaves.bat[57]

---

[54] See Control Data Tab of Section 3.8.4.1 for details.

[55] This file is created for users to start BeoPEST master manually.

[56] This batch file starts an instance of BeoPEST agent.

[57] This batch file starts all instances of BeoPEST agent.

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