GMS User Manual, vol. 3

Models and Modeling

Contents

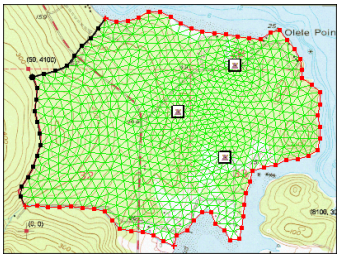
Articles

References

6. Models

6.1. FEMWATER

FEMWATER

FEMWATER	
 *FEMWATER Screenshot*	
Model Info	
Model type	3D mesh, finite-element, Steady state and transient
Developer	George Yeh
Documentation	FEMWATER Manual [1]
Tutorials	FEMWATER Tutorials

GMS includes a graphical interface to the groundwater model FEMWATER. FEMWATER is a 3D finite element, saturated/unsaturated, density driven, flow and transport model. FEMWATER was originally written by G.T. (George) Yeh at Penn State University (Yeh, et. al., 1992). The version of FEMWATER that is supported by GMS is a special version that has been modified by G.T. Yeh and the U.S. Army Engineer Waterways Experiment Station. This version is a coupled version of the original FEMWATER model (which solved for flow only) with the transport model LEWASTE (also developed by George Yeh).

A separate reference manual is available which describes the new version of FEMWATER in detail (Lin, et. al., 1997). This manual contains a description of the input requirements and should be read completely before using GMS to set up a problem.

Pre-Processing

- Building a FEMWATER Model
- FEMWATER Model Input
- Saving a FEMWATER Simulation

Post-Processing

- FEMWATER Display Options
- FEMWATER Post Processing Viewing Options

External Links

- Mar 2004 ERDC/CHL CHETN-XI-1 DDJC-Sharpe Defense Distribution Depot: FEMWATER 3D Transport Model of TCE Plume Migration with Natural Attenuation [2]

References

[1] http://gmsdocs.aquaveo.com/Femwater.pdf
[2] http://chl.erdc.usace.army.mil/library/publications/chetn/pdf/chetn-xi-1.pdf

FEMWATER Commands

Menu Command	Description
New Simulation...	Opens a dialog to start a new FEMWATER model.
Delete Simulation...	
Check Simulation...	Opens a dialog to run a check of the model to verify that all necessary inputs are present and working for the model to run.
Run FEMWATER...	
Read Solution...	
Geometry File...	
Titles...	
Run Options...	
Initial Conditions...	
Iteration Parameters...	
Particle Tracking...	
Time Control...	
Output Control...	
Fluid Properties...	
BC Display Options...	
Variable BC Options...	
Assign Node/Face BC...	
Point Source/Sink BC...	
Delete BC	

6.1.1. FEMWATER Pre-Processing

Building a FEMWATER Model

Three various approaches provided in GMS for constructing a FEMWATER model. The model can be completely defined using the tools in the 3D Mesh module (the direct approach), or the model can be defined with the aid of the feature object tools in the Map module (the conceptual model approach). A horizons to 3D mesh approach can also be used.

Basic Steps in Building a FEMWATER Model

The basic steps in building a FEMWATER model include:

- Build a 3D mesh defining the extents of the model. Three approaches are available:
  - FEMWATER Direct Approach
  - FEMWATER Conceptual Model Approach
  - Horizons to 3D Mesh
- Initialize FEMWATER
- Assign boundary conditions and model stresses, including sources and sinks
  - Point Source/Sink BC (Wells)
  - Assign Node/Face BC
- Assign material properties
- Run FEMWATER

FEMWATER Direct Approach

The Direct Approach

For models with simple geometry and boundary conditions, the entire model can be constructed using the tools and commands in the 3D Mesh module. With this approach, the editing of the FEMWATER data is performed directly on the nodes and elements of the mesh. The first step is to create a 3D mesh covering the model domain using the mesh building tools in the 3D Mesh module. The boundary conditions and source/sink terms are then assigned by selecting nodes, elements, and element faces and assigning values directly to the selected objects. The model is then saved and FEMWATER is launched.

Creating a Mesh

The first step in performing a FEMWATER simulation is to create a 3D finite element mesh. The volumetric domain to be modeled by FEMWATER is idealized and discretized into hexahedra, prisms, tetrahedra, and or pyramids. Elements are grouped into zones representing hydrostratigraphic units. Each element is assigned a material ID representing the zone to which the element belongs. When constructing a mesh, care should be taken to ensure that elements do not cross or straddle hydrostratigraphic boundaries.

The tools provided in GMS for constructing a 3D finite element mesh are provided in the 3D Mesh Module. When constructing a mesh for FEMWATER, there are a few important guidelines that should be considered. These guidelines are described in Chapter 3 of the FEMWATER Reference Manual.

The most efficient method for constructing a 3D mesh for FEMWATER is to use the conceptual model approach. The FEMWATER conceptual model can be used to automatically build a 2D mesh that matches the

model boundaries and is refined around wells. This mesh can then be extruded into a 3D mesh.

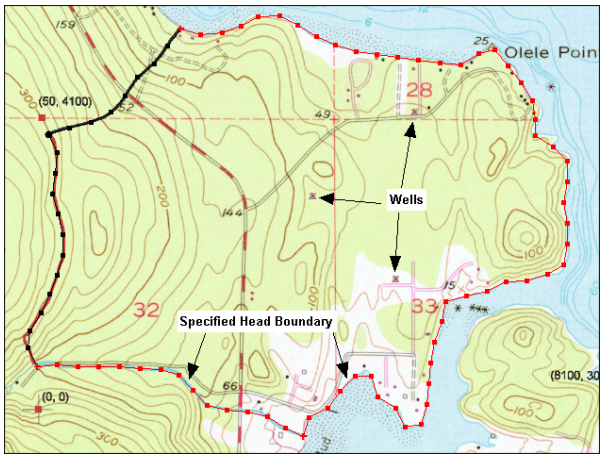
Solids can also be used to make a structured mesh. This is accomplished with the Solids -> Layered Mesh command in the ***Solids*** menu.

FEMWATER Conceptual Model Approach

The preferred method for setting up a FEMWATER simulation is to use the feature object tools in the Map module to define a FEMWATER conceptual model of a site being studied. The conceptual model is a high-level description of the site including sources/sinks, the boundary of the domain to be modeled, rainfall and seepage zones, and material zones within each of the layers. The conceptual model is defined with feature objects, including points, arcs, and polygons, and is constructed independently of a numerical grid. Once the conceptual model is complete, a mesh is automatically constructed to fit the conceptual model, and the FEMWATER data are converted from the conceptual model to the nodes, elements, and element faces. The dialogs and interactive editing tools in the FEMWATER menu can then be used to edit or review the data if desired.

A FEMWATER model can be created in GMS using one of two methods: assigning and editing values directly to the nodes and elements of a mesh (the direct approach), or by constructing a grid-independent representation of the model using feature objects and allowing GMS to automatically assign the values to the nodes and elements (the conceptual model approach). Except for simple problems, the conceptual model approach is typically the most effective.

The conceptual model approach utilizes feature objects in the Map module. A FEMWATER conceptual model is created in the Map module and feature objects are used to create a high level representation of the site you are modeling. The figure below shows a sample conceptual model.



Sample FEMWATER Conceptual Model

Two Step Process

A FEMWATER conceptual model is used to build a numerical model using a two step process. In the first step, a 3D mesh is created. This can be done by using the feature objects in conjunction with a set of TINs to build a 3D Mesh or a solid can be converted to a layered 3D Mesh using the ***Solids → Layered Mesh*** command. In the second step, the boundary conditions and recharge values assigned to the feature objects are automatically assigned to the appropriate nodes and element faces of the 3D mesh using the ***Feature Objects | Map → FEMWATER*** command.

To create a FEMWATER conceptual model right click on the Map Data folder in the Project Explorer and select the ***New Conceptual Model*** command. In the *Conceptual Model Properties* dialog change the model type to FEMWATER in the pull-down list. In the dialog the simulation options of flow and transport can also be toggled on or off. Next create a coverage by right clicking on the FEMWATER conceptual model in the data tree and selecting

New Coverage. The coverage attributes can then be setup in the *Coverage Setup* dialog.

A FEMWATER coverage can contain points, arcs, and polygons. The points are used to define wells, the arcs are used to define boundary conditions, and the polygons are used to define recharge zones. In most cases, a single coverage is sufficient. However, multiple FEMWATER coverages can be used if desired.

More on point/arc properties here: FEMWATER Point / Arc Properties

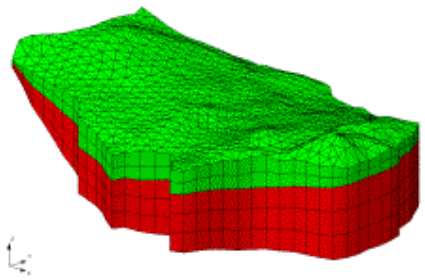
Build a 3D Finite Element Mesh

Once the FEMWATER conceptual model is constructed, the next step is to use the conceptual model to build a 3D finite element mesh. This is accomplished by first building a 2D mesh, then building the 3D mesh by extruding each of the 2D elements in 3D elements.

Map → 2D Mesh

The first step in building the 3D mesh is to select the *Feature Objects* | *Map → 2D* Mesh command. This command creates a 2D mesh by automatically filling in the interior of the conceptual model with nodes and elements. The size and spacing of the elements is controlled by the spacing of the vertices on the arcs and by the refine point attribute assigned to any wells in the interior of the conceptual model.

An example of the ***Map → 2D Mesh*** command is shown in the following figure. A sample FEMWATER conceptual model is shown in part a. The 2D mesh resulting from execution of the ***Map → 2D Mesh*** command is shown in part b.



Converting a FEMWATER Conceptual Model (a) Conceptual Model (b) 2D Mesh Created with *Map → 2D Mesh Command* (c) 3D Mesh Created by Extruding 2D Mesh (d) 3D Mesh after *Map → FEMWATER* Command.

Creating the 3D Elements

Once the 2D mesh is created, the next step is to create the 3D mesh by extruding each of the 2D elements into a series of 3D elements. The elevations of the 3D elements can be defined from a set of boreholes, a set of TINs, or a set of Solids.

For sites with relatively simple stratigraphy, the ***Regions → 3D Mesh*** command in the Borehole module can be used.

For sites with more complex stratigraphy, the ***TINs → 3D Mesh*** command in the TIN module should be used.

A mesh can also be created using the ***Solids → Layered Mesh*** command in the Solid module.

FEMWATER Flows

Computed flows can be automatically summed and displayed for FEMWATER simulations. To enable this option, the Save flux file option must be selected in the *FEMWATER Output Control* dialog prior to saving the FEMWATER model. When this option is selected, FEMWATER saves a lumped nodal flow data set file as part of the FEMWATER solution. This file is automatically read into GMS as part of the FEMWATER solution.

Once a FEMWATER flux file has been read into memory as part of a FEMWATER solution, the computed flux through a set of nodes can be displayed simply by selecting the nodes. The flow budget (in, out, net) for the selected nodes is displayed in the ***Status Bar*** at the bottom of the GMS window. The flow budget is only displayed if the active solution is a FEMWATER solution.

It should be noted that lumped nodal fluxes are only non-zero for boundary nodes where a boundary condition has been assigned.

Point Source/Sink BC

The ***Point Source/Sink BC*** command is used to assign a flow rate to a node. This option is typically used to assign flow rates to interior nodes to simulate injection or extraction wells. When a point source/sink is first assigned to a node, the node should be selected with the ***Select Nodes*** tool. The ***Point Source/Sink BC*** command is then selected and the *Point Source/Sink BC* dialog appears. Both a flow rate and a concentration may be specified at a point source/sink node. The values can be constant or transient.

Existing boundary conditions can be deleted by selecting the boundary condition with the ***Select Boundary Nodes***, ***Select Boundary Faces***, or ***Select Wells*** tool and selecting the ***Delete BC*** command from the *FEMWATER* menu.

The Select Well Tool

When a point source/sink boundary condition is applied to a node, a well symbol is placed on the node. The ***Select Wells*** tool can then be used to select the node rather than the ***Select Nodes*** tool whenever the well needs to be edited or deleted. The ***Select Wells*** tool is easier to use than the ***Select Nodes*** tool when there are a large number of nodes since it only selects nodes with point source/sink boundary conditions.

Assign Node/Face BC

The ***Assign Node/Face BC*** command in the *FEMWATER* menu is used to either assign a new boundary condition or edit an existing boundary condition to a selected set of boundary nodes or boundary element faces. The dialog that appears depends on whether nodes or faces are selected.

Nodal Boundary Conditions

If a set of nodes is selected when the ***Assign Node/Face BC*** command is selected, the Node BC dialog appears. Boundary conditions assigned to nodes correspond to Dirichlet boundary conditions. Both head and concentration can be specified.

Head

Head boundary conditions in FEMWATER are assigned as total head. FEMWATER converts the total heads to pressure heads internally. Heads can be specified as a constant value or as a transient value (curve of head vs. time).

The Load Data Set button can be used to assign the head values from a data set. For example, if the Elevation data set is selected, the head is set equal to the node elevation at each of the selected nodes.

Concentration

The concentration can also be specified as either a constant or transient value. Since the concentration is a Dirichlet boundary condition, it represents a fixed concentration at the node. It does not represent the concentration of the incoming fluid.

Face Boundary Conditions

If a set of faces is selected when the ***Assign Node/Face BC*** command is selected, the Face BC dialog appears. Boundary conditions assigned to faces are flux-type boundary conditions. Both flux and concentration can be assigned independently. In both cases, the type must be designated as either Variable, Flux (Cauchy), or Flux gradient (van Neumann). The value can be defined as a constant or transient value.

Existing boundary conditions can be deleted by selecting the boundary condition with the Select Boundary Nodes, Select Boundary Faces, or Select Wells tool and selecting the ***Delete BC*** command from the *FEMWATER* menu.

FEMWATER Point / Arc Properties

Point Properties

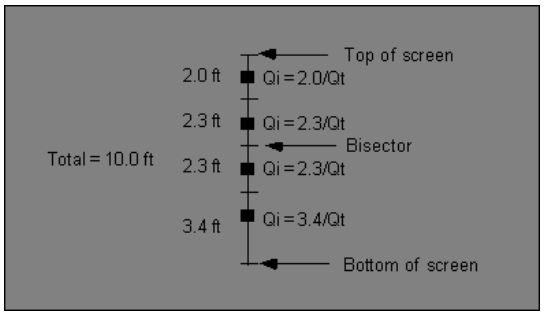
Points in a FEMWATER coverage are used to define injection and extraction wells. The point attributes are edited via the *Point Properties* dialog. The Point Attributes dialog is accessed by selecting a point(s) and then selecting the Attribute Table command in the coverage right click option menu. Each point's properties are displayed in the spreadsheet. The options in the dialog are as follows.

Type - The type of point can be changed to either a well or an observation point. These options are available depending on what was selected in the *Coverage Setup Dialog*. The type for each point is defaulted to "NONE" in the **Type** column pull-down list.

Refine - If the Refine mesh around point option is selected, the edge length of the elements surrounding the node are set to the size entered in the Element size edit field when the 2D projection mesh is generated. (see: Map -> 2D Mesh)

Wells - To define a point as a extraction or injection well change the **Type** to "well" in the spreadsheet. For each well, a flow rate and a concentration can be assigned. Each well is also assigned a the top and bottom elevation of the screened interval.

The screened interval is used to determine which of the nodes in the 3D mesh are used to represent the well in the numerical model. When the ***Map -> FEMWATER*** command is selected, all nodes intercepted by the well screen are found and each node is marked as a point source/sink (a well node). The flow assigned to the well in the conceptual model is distributed to the mesh nodes using the logic illustrated below. A length of influence on the well screen is found for each node and the flux assigned to the node is proportional to the length of influence divided by the total screen length.



The Distribution of Flux Rate to Nodes Overlapped by Well Screen.

Arc Properties

Arcs in a FEMWATER coverage are used to define the model boundary and the boundaries of recharge zones. Arcs on the outside boundary of the model can also be used to specify boundary conditions. Boundary conditions are assigned using the FEMWATER Arc Properties dialog. The Arc Properties dialog is accessed selecting the ***Attribute Table*** command in the coverage right click option menu. The options for arc attributes are as follows:

Flow bc - The Flow bc option is used to define a specified head or specified flux boundary. If this option is selected in the drop-down list. The available options are:

- **Specified head** - If this option is selected, a head value is assigned to each of the two nodes at the endpoints of the arc. If the two values at the endpoints are different, the head is assumed to vary linearly along the arc length. When the ***Map -> FEMWATER*** command is selected, all nodes on the boundary of the mesh beneath the arc are found and the nodes are marked as specified head nodes. A linearly interpolated head value is

assigned to each node.

- **Specified flux** - If this option is selected, a flux value is assigned to the arc in the Flux rate column of the spreadsheet. When the ***Map -> FEMWATER*** command is selected, all vertical element faces on the boundary of the mesh beneath the arc are found and the specified flux rate is assigned to the faces.
- **Variable flux** - If this option is selected, a flux value is assigned to the arc. When the ***Map -> FEMWATER*** command is selected, all vertical element faces on the boundary of the mesh beneath the arc are marked as variable boundary faces. If a flux value of zero (the default value) is assigned, the element faces represent a seepage face boundary where below the water table, the head is set equal to the elevation.

Contaminant - The Contaminant option is used to model concentration or mass flux boundary conditions. This option is selected in the Transport bc column in the spreadsheet. The available options are:

Specified concentration - If this option is selected, a concentration value is assigned to the arc using the Concentration flux column. When the ***Map -> FEMWATER*** command is selected, all mesh nodes on the boundary of the mesh beneath the arc are found and the specified concentration is assigned to the nodes.

Specified mass flux - If this option is selected, a mass flux value is assigned to the arc using the Mass flux column. When the ***Map -> FEMWATER*** command is selected, all vertical element faces on boundary of the mesh beneath the arc are found and the specified mass flux rate is assigned to the faces.

Variable (concentration) - If this option is selected, a concentration value is assigned to the arc using the Concentration column. When the ***Map -> FEMWATER*** command is selected, all element faces on the boundary of the mesh beneath the arc are found and the specified concentration is assigned to the faces as a variable type boundary condition. Note that this boundary condition can be used in conjunction with any of the three options for specified head/fluid flux. The proper use of this type of boundary condition is explained in the FEMWATER Reference Manual [1].

Assigning to Zones - The zone column is used to determine how the boundary conditions are applied to the nodes and element faces when the ***Map -> FEMWATER*** command is selected. By default, the boundary conditions are assigned to all nodes and element faces beneath the arc. However, in some cases it is useful to restrict the boundary condition to only a portion of the vertical boundary beneath the arc. This can be accomplished by selecting the Selected zones only option and marking the material zones where the boundary condition is to be applied.

Node Properties - As explained in the previous section, if an arc is marked as a specified head arc, a head value must be assigned to the two nodes at the endpoints of the arc. This is accomplished using the FEMWATER Node Attributes dialog. The Arc Properties dialog is accessed by selecting a node and then selecting the Attribute Table command in the coverage right click option menu. If the head values assigned to the two endpoints of an arc are different, the head is assumed to vary linearly along the length of the arc.

Polygon Properties - Polygons in a FEMWATER coverage serve two purposes: they define the model domain and they can be used to assign recharge values on a zonal basis. When building a FEMWATER coverage, the boundary of the model domain should be delineated using arcs. In order to use the coverage to build a 3D mesh, the arcs should be used to build one or more polygons defining the model domain using the Build Polygon command.

In addition to defining the model domain, a material ID and a recharge value can be assigned to polygons in the FEMWATER coverage using the Polygon Properties dialog. The polygon attributes are as follows:

Material - The Material pull-down list can be used to associate a material with a polygon. When the ***Map -> 2D Mesh*** command is selected, all 2D elements within the polygon are assigned the specified material. This material can be used to define the material type for the 3D elements when the 2D elements are extruded using the ***Fill Between TINs -> 3D Mesh*** command.

Fluid Flux - The Fluid flux option is used to assign a specified flux to the polygon. The flux can be assigned using either the Specified flux or Variable flux options. These optins are set in the *Flow bc* drop-down list. When the ***Map -> FEMWATER*** command is selected, all element faces on the top of the 3D mesh inside the polygon are found and the specified flux is assigned to the element faces.

Contaminant - The Contaminant option is used to assign a mass flux or a concentration. If the Specified mass flux option is selected, the specified mass flux rate is assigned to all element faces on the top of the mesh when the ***Map -> FEMWATER*** command is selected. If the Variable (concentration) option is selected, the specified concentration is assigned to all element faces inside the polygon.

FEMWATER Model Input

Several model parameters must be defined for a given FEMWATER simulation. In many cases the default values suffice. The following is a list of the required parameters:

Titles

The ***Titles*** command in the *FEMWATER* menu is used to enter two sets of titles. Each set contains three lines of text. The first set is written to the top of the geometry file when the simulation is saved. The second set is written to the top of the model file.

- ***Run Options*** - This command in the *FEMWATER* menu brings up the Run Options dialog. This dialog is used to enter a set of general analysis options.

  Type of Simulation - Three options are available for designating the type of simulations to be performed by FEMWATER:

  Flow only - This option is used to perform a steady state or transient flow simulation.

  Perform a transport simulation only - For this case, a steady state or transient flow simulation must be performed prior to the transport simulation. The results of this simulation (velocity and moisture content) are then input to FEMWATER as a flow solution initial condition.

  Coupled flow and transport - With a coupled flow and transport simulation, either density-dependent flow or density-independent flow can be simulated. This option is controlled by entering the appropriate parameters defining the relationship between concentration and density and concentration and viscosity. These parameters are entered in the *Fluid Properties* dialog.

  Steady State vs. Transient - FEMWATER can be run in either a steady state or transient mode. The steady state mode is only allowed when the Flow only option has been selected.

  Units - The Units button brings up the Units dialog. This dialog is used to enter the units for length, time, concentration, etc. for the simulation. GMS uses the selected unit options to display the appropriate units next to each input edit field in the other FEMWATER dialogs.

  Other Options - The remaining run options are described in the FEMWATER Reference Manual. In most cases, the default values are appropriate.

- FEMWATER Initial Conditions

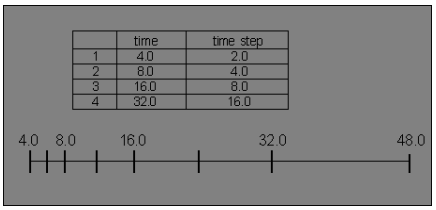
Iteration Parameters

Brings up the Iteration Parameters dialog. This dialog is used to enter the iteration parameters for each simulation type (flow only, transport only, coupled flow and transport).

Particle Tracking Parameters

The Particle Tracking dialog is used to edit parameters relating to how the particle tracking is carried out by FEMWATER during the transport phase.

Time Control Parameters



Time-Line Of Computational Time Steps Defined Using the Variable Time Step Option and the XY Series Editor.

The Time Control dialog is used to enter the data used by FEMWATER to compute the computational time intervals. It is also used to define the reference time. The options in the dialog are as follows:

Time Steps

There are two methods for defining the computational time steps: Constant time step and Variable time step. With the Constant time step method, the first time step is assumed to begin at time 0.0. A constant interval time is entered along with a maximum simulation time. For example, if a constant time step of 2.0 is defined along with a maximum simulation time of 10.0, six computational time steps will be defined at 0.0 (the initial condition), 2.0, 4.0, 6.0, 8.0 and 10.0.

The Variable time step option permits variable intervals between time steps. Selecting the Variable Times button brings up the XY Series Editor. The XY Series Editor has one column for entering times and another for entering time steps. In the time column, the absolute time for a computational time step should be entered. The time step corresponding to each time represents the interval to be used from one specified time to the next.

A simple example of times and time steps defined in the XY Series Editor and the resulting computational time steps to be used by FEMWATER is shown below. In this case the maximum simulation time is equal to 48.0.

Output Control

The Output Control dialog is used to enter parameters defining what type of output will be printed or saved from FEMWATER.

Printed Output File

The left side of the dialog controls what information is written to the printed output file. The printed output file is an ASCII file where the solution will be written.

Data Set Files

The results of a FEMWATER solution are GMS data set files. The Data set files portion of the dialog permits specification of what data sets will be saved and at what frequency. The solution data set files are used as input to GMS to graphically visualize the results. ASCII or binary solution file formats may also be specified. In most circumstances, binary solution files should be specified, since they take up less memory and can be read more quickly by GMS.

Fluid Properties

The ***Fluid Properties*** command in the *FEMWATER* menu brings up the *Fluid Properties dialog*. This dialog is used to specify the acceleration of gravity and the density, viscosity, and compressibility of the fluid.

The **Edit Values** button brings up the *FEMWATER Fluid Coefficients* dialog. This button is undimmed when transport is being analyzed as part of the simulation.

Material Properties

As a 3D finite element mesh is constructed in GMS, a list of materials is defined and each element in the 3D mesh has a material type associated with it. The list of materials is initially created using the *Materials* dialog accessed through the *Edit* menu.

- *Kxx, Kyy, Kzz, Kxy, Kxz, Kyz* - The hydraulic conductivity tensor is defined via the Kxx, Kyy, Kzz, Kxy, Kxz, Kyz fields. Since the tensor is symmetric only the upper right half of the matrix can be specified.

Hydraulic Conductivity Tensor

Kxx	Kxy	Kxz
Kyx	Kyy	Kyz
Kzx	Kzy	Kzz

- *Moisture Content, Relative Conductivity, Water Capacity curves* - These unsaturated zone curves must be defined for each material. The curves can be defined using either the XY Series Editor or the Curve Generator (discussed below). The Curve Generator is accessed via the **Generate Unsat Curves** button in the bottom of the dialog. When that button is selected, the curves that are generated will be associated with the active material, or the material in the spreadsheet row that currently has the focus.

Curve Generator

In most cases, the simplest way to generate a set of pressure head curves for the unsaturated zone is to use the *Curve Generator*. The **Generate Unsat Curves** button brings up the *Curve Generator* dialog. This dialog is used to automatically generate a set of unsaturated zone curves using the van Genuchten equations described in the FEMWATER Reference Manual. The items in the top of the dialog are used to select the curve type ('linear front' or 'van Genuchten equation') and the max height of capillary rise above the water table. Two methods are available for entering the Van Genuchten parameters: (1) you can select the Manual parameter input option and enter the values directly, or (2) you can select the Preset parameter values option and choose from a list of pre-defined soil types.

Once the parameters are defined the **Compute Curves** button can be used to generate a set of curves. The curves are displayed in the bottom of the dialog. New values can be entered and the process can be repeated until a satisfactory result is obtained. When the OK button is selected, the active curves are assigned to the current material.

Each of the unsaturated zone curves is a piece-wise linear curve defined by a sequence of points. The number of points in each curve is either specified by the user or determined automatically by specifying a *Max percent change*. If the **max percent change** option is used, a new point is added to the curve each time the parameter changes by the Max percent value.

Note that the effective porosity for each material is defined from the pressure head vs. moisture content curve. The value at p = 0 is taken from the curve and is written to the model file as part of the MP2 card.

Note also that GMS assumes that the van Genuchten 'alpha' value is entered in units consistent with the current model units. GMS displays the current model units next to the input field to help you remember this.

FEMWATER Initial Conditions

Whenever a FEMWATER analysis is performed, a set of initial conditions must be defined. Initial conditions define the initial status of the pressure head and concentration. Three types of initial conditions are possible for a FEMWATER simulation: cold starts, hot starts, and flow solutions. Cold starts are used to establish a set of initial values at the beginning of a steady state or transient simulation. Hot starts are used to continue a previous run of FEMWATER without having to start over from the beginning. Flow solutions are used to define the flow field that is necessary when performing a transport only simulation (as opposed to coupled flow and transport). Initial conditions are described in more detail in Chapter 7 of the FEMWATER Reference Manual.

Initial conditions are defined using the Initial Conditions dialog. The available options are as follows:

Cold Starts

If a flow only simulation is performed, a set of pressure heads is required for the cold start initial condition. If a transport only simulation is performed, a set of concentrations is required (in addition to the flow solution as explained below). If a coupled flow and transport simulation is being performed, both heads and concentrations are required.

Pressure Head

Two options are available for designating a pressure head cold start initial condition. One option is to enter a constant value into the field labeled Total head. This essentially defines an initial condition corresponding to a flat water table. FEMWATER reads this value and internally generates an array of pressure heads by subtracting the nodal elevations from the given total head value.

The Read from data set file option can be used to designate that the pressure head varies spatially and that the values will be read from a data set file. If this option is selected, the name of the file must be entered at the bottom of the Initial Conditions dialog in the field titled IC pressure head. The data set file is a standard GMS data set file in either the ASCII or binary format. The data set file can be generated using the interpolation options and then saved using the ***Export Data Set*** command accessed by right-clicking on the data set file. However, a simpler approach to generating a well-posed initial condition is to use the **Generate I.C.** button. This button brings up the *Generate Pressure Head Initial Condition* dialog.

The first two items in the *Generate Pressure Head Initial Condition dialog* are used to select a 2D scatter point set and data set. The scatter point set defines a set of elevations corresponding to a best estimate of the final computed water table elevation. A minimum pressure head may also be entered. When the **OK** button is selected, the elevations in the scatter point set are interpolated to the nodes of the 3D mesh. This defines a total head initial condition. The pressure head initial condition is computed by subtracting the node elevations from the total heads. The user is then prompted for a file name and the pressure head data set is saved to a GMS data set file and the path to the file is automatically written to the IC pressure head field at the bottom of the Initial Conditions dialog.

The pressure head cold start can have a significant influence on the speed of convergence. In some cases, a poorly defined initial condition may even prevent convergence. In most cases, the Read from data set file/Generate IC option should be used since it results in a better initial condition.

Concentration

When defining a set of concentration values for a cold start initial condition, it is often useful to use a constant value of concentration everywhere in the problem domain. For example, in many cases, an initial condition of zero concentration everywhere in the problem domain is appropriate. The Use constant value option can be used to easily define a constant concentration for the entire mesh. If a constant value is not appropriate, the Read from data set file option should be chosen. In this case, the initial condition varies spatially and the values are defined by a data set file. This file can be created by interpolating concentrations to the mesh and saving the resulting data set to a file using the Export command in the Data Tree. When this option is chosen, the name of the data set file containing the concentration initial condition is entered in the IC Concentration field at the bottom of the Initial Conditions dialog.

Hot Start

Hot starts are used to begin a new simulation starting at a given time step of a solution computed from a previous transient simulation. If the hot start option is chosen, FEMWATER reads the specified hot start file and finds the time step corresponding to the specified time. The solution then begins using the data set at that time as the initial condition.

The solution files necessary for a hot start depend on the type of simulation. If a flow only simulation is being performed, a pressure head file is required. If a transport only simulation is being performed, a concentration file is required (in addition to the flow solution described below). If a coupled flow and transport simulation is being performed, both pressure head and concentration are required. When the Hot start option is chosen, the names of the files used for the hot start are entered in the fields at the bottom of the Initial Conditions dialog.

If the Hot start option is chosen, the Append to moisture content file and Append to velocity file options may be selected. If these options are selected, the name of previously computed moisture content and velocity files can be specified in the FEMWATER super file. The file can be edited using a text editor. The super file format is described in the FEMWATER Reference Manual. FEMWATER opens these files and appends the new moisture content and velocity values to the files after the designated hot start time.

Initial Condition File Format

For both the cold and hot start options, data set files can be used to specify the initial conditions. These files can be saved in either ASCII or binary. The format of the files can be specified in the Initial condition file format section. All initial condition files should be either ASCII or binary, i.e., the types cannot be mixed for a given simulation. If the Generate IC button is used to create the pressure head file, the ASCII option should be selected.

Flow Files

A third type of initial condition is required when a transport only simulation is being performed. A transport only simulation utilizes a previously computed flow solution (steady state or transient) to define the three-dimensional flow field required to properly model the contaminant migration. The flow solution consists of a pressure head file.

The flow solution for a transport only simulation is used in combination with either a cold start or a hot start. With a cold start, a set of initial concentration values is provided for concentration in addition to the steady state or transient flow solution. With a hot start, a transient concentration solution and a hot start time is provided in addition to the flow solution.

When a transport only option is selected, the name of the pressure head file from the flow solution is entered at the bottom of the Initial Conditions dialog. The Flow file format options in the Initial Conditions dialog are used to specify whether these files are ASCII or binary, and whether they are steady state or transient.

Saving a FEMWATER Simulation

Once a FEMWATER simulation has been set up and checked for errors, the final step before running the model is to save the simulation. FEMWATER simulations are saved using the ***Save*** and ***Save As*** commands in the *File* menu.

Selecting the ***Save*** command saves the GMS project including the model simulation. By default the model simulation will be saved to the same location as the GMS project. However, in the Save dialog the path for the model simulation can be specified.

A FEMWATER simulation is actually saved to a set of input files. The FEMWATER super file is a special type of file which is used to organize the set of files used in a simulation. The names of all of the input and output files associated with a simulation are saved in the super file. When FEMWATER is launched, the name of the super file is automatically passed to the FEMWATER executable.

When a FEMWATER simulation is saved, the names of the other FEMWATER input files are automatically patterned after the name of the super file. For example, if the super file is named sampmod.fws, the other files are named sampmod.geo, sampmod.3bc, etc.

Geometry File Options

When a FEMWATER simulation is saved using the ***Save*** or ***Save As*** command, all data associated with the simulation is saved to disk, including both the mesh geometry and the boundary conditions. For large FEMWATER models, the mesh file can take up a substantial amount of disk space and take a long time to save. During a model exercise, it is often the case that multiple versions of the simulation are saved to disk where the only change from one simulation to the next is changes in the analysis options or boundary conditions. In such cases, both time and disk space can be saved by re-using the same geometry file from one run to the next. This can be accomplished by first saving a copy of the FEMWATER simulation to disk and then selecting the ***Geometry File*** command in the *FEMWATER* menu. This command brings up the Geometry File dialog. If the Use existing geometry file option is selected, the Browse button can be used to identify the previously saved geometry file. Once this option is selected, each time GMS saves the FEMWATER super file, it does not re-save the geometry file. Rather, it saves the path to the specified geometry file.

6.1.2. FEMWATER Post-Processing

FEMWATER Display Options

The properties of all FEMWATER boundary conditions that GMS displays on the screen can be controlled through the FEMWATER tab of the *Display Options* dialog. This dialog is opened by right clicking on the 3D Mesh Data entry in the Project Explorer, selecting the Display Options command, and then selecting the FEMWATER tab. This tab is only visible when there is a FEMWATER simulation. It can also be accessed from the from the Display menu, the *FEMWATER* menu, or the Display Options macro. The following table describes the display options available for the FEMWATER model.

Display Option	Description
Well	Controls the display of well boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Well (super pump node)	Controls the display of well super pump nodes boundary conditions. The fill color can be adjusted using the button to the left of the display toggle.
Well conc.	Controls the display of well concentration boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Variable	Controls the display of variable boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Variable conc.	Controls the display of variable concentration boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Head	Controls the display of head boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Head conc.	Controls the display of head concentration boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Flux	Controls the display of flux boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Flux conc.	Controls the display of flux concentration boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Grad. flux.	Controls the display of gradient flux boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Grad. flux. conc.	Controls the display of gradient flux concentration boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
BC values	Controls the display of boundary condition values. The font, font size, and font color can be adjusted using the button to the left of the display toggle.
Display symbol legend	Controls the display of a legend containing the symbols for the boundary conditions used in the FEMWATER simulation.
Check All	By clicking this button, all of the display options are turned on.
Check None	By clicking this button, all of the display options are turned off.

FEMWATER Post Processing Viewing Options

Part of the output from FEMWATER is a set of files representing velocity, moisture content, pressure head, and concentration. These files are written in the standard GMS data set file format and can be imported directly to GMS using the ***Read Solution*** command in the *FEMWATER* menu.

Once the FEMWATER solution data sets have been imported to GMS, the standard GMS visualization tools can be used to generate vector plots, cross sections, iso-surfaces, and animations.

One of the output options for FEMWATER is a flux file containing flow budget data for boundary nodes. Once this file is imported, FEMWATER fluxes for selected nodes can be viewed.

Particle Tracking

Particle tracking can be done with a FEMWATER solution, similar to using MODPATH to do particle tracking with a MODFLOW solution. For more information:

- FEMWATER Particle Sets

Flow / Flux

Computed flows can be automatically summed and displayed for FEMWATER simulations. To enable this option, the Save flux file option must be selected in the *FEMWATER Output Control* dialog prior to saving the FEMWATER model. When this option is selected, FEMWATER saves a lumped nodal flow data set file as part of the FEMWATER solution. This file is automatically read into GMS as part of the FEMWATER solution.

Once a FEMWATER flux file has been read into memory as part of a FEMWATER solution, the computed flux through a set of nodes can be displayed simply by selecting the nodes. The flow budget (in, out, net) for the selected nodes is displayed in the **Status Bar** at the bottom of the GMS window. The flow budget is only displayed if the active solution is a FEMWATER solution.

It should be noted that lumped nodal fluxes are only non-zero for boundary nodes where a boundary condition has been assigned.

FEMWATER Particle Sets

Particle tracking can be done with a FEMWATER solution, similar to using MODPATH to do particle tracking with a MODFLOW solution. Particle starting locations can be automatically generated at wells, or at element or element face centroids by using the the commands in the Particle Tracking menu. Once the starting locations are created, the pathlines are automatically computed. Particles are grouped into particle sets, just like with MODPATH.

Restrictions

In order to compute the pathlines, the FEMWATER solution must contain nodal velocity, and nodal moisture content data sets. You can tell FEMWATER to create these data sets using the Output Control dialog. Also, the effective porosity ratio for all materials must be non-zero.

Particle tracking is steady state only. That is, the particles are only influenced by the active time step.

Particles are currently not tracked correctly through hexahedron elements. If you refine the hex elements to create wedges, the particles will be tracked correctly.

Display Options

A set of display options associated with FEMWATER particle tracking is provided in GMS. These options are accessed through the Display Options command in the Particle Tracking menu. This command is only available if a FEMWATER simulation exists. This command brings up the Particles tab of the 3D Mesh Display Options dialog. The following table describes the display options available for the particle tracking.

Display Option	Description
Starting locations	The starting locations for the particles can be turned on and off. The symbol style, color and size can also be adjusted.
Starting location indices	The starting locations indices for the particles can be turned on and off. The font style, color and size can also be adjusted.
Ending locations	The ending locations for the particles can be turned on and off. The symbol style, color and size can also be adjusted.
Pathlines	The pathlines can be toggled on and off, and the pathline style and color can be adjusted. The pathline color can be set to the default color, or the color corresponding to the starting or ending zone codes of the pathlines.
Direction arrows	Direction arrows can be displayed along the pathlines. The size of the arrow heads can be set by specifying the Length in pixels. The arrows are displayed along the pathline at an interval corresponding to the Length specified.
Auto-update	The auto-update can be turned off and on, and controls the automatic updating of the particles.

6.2. MODAEM

MODAEM

MODAEM	
Model Info	
Model type	Analytic element, Steady state analysis
Developer	Vic Kelson of Wittman Hydro Planning Associates
Tutorials	MODAEM Tutorials

MODAEM is an analytic element model developed by Vic Kelson of Wittman Hydro Planning Associates (WHPA) of Bloomington, Indiana. The key feature of analytic element models is that they do not require the discretization of the interior of the model domain into cells and elements as is the case with finite difference and finite element models. Rather, the model is defined by “analytic elements” representing line sources and sinks such as rivers and drains or specified head and specified flow boundaries. Wells are also represented as points, and recharge and aquifer properties can be defined on polygons. MODAEM then formulates a set of equations based on these entities and the equations can be solved for any location in the horizontal plane.

MODAEM is perfectly suited for the conceptual model approach used by GMS since the input data to MODAEM is consistent with the GIS feature objects (points, arcs, and polygons) used to define a GMS conceptual model. In other words, once a MODAEM conceptual model is defined, the model can be immediately executed. There is no need to build a grid or mesh. A background grid is utilized for displaying the MODAEM results using contour lines. However, the background grid is purely for visualization purposes and has nothing to do with the accuracy of the model. MODAEM also supports particle tracking/streamlines.

One of the caveats of the analytical element approach is that a simplified representation of the aquifer must be used. The aquifer properties (K, porosity, bottom elevation, aquifer thickness) can be assigned to polygons, but they are assumed to be constant within each polygon. Currently MODAEM supports steady, confined and unconfined two-dimensional groundwater flow, although streamlines are computed in three dimensions.

Linking MODAEM and MODFLOW

GMS also includes a feature to link MODAEM models with MODFLOW models. The main application of this linkage is for defining boundary conditions for a local scale model. A regional model can be built with MODAEM and then linked to a local scale MODFLOW model. This is accomplished as follows:

1. Build and calibrate the regional scale model using MODFLOW.
2. Build a conceptual model for the local scale MODFLOW model. When setting up the coverage properties for the source/sink coverages, be sure to toggle on the **MODAEM Head** and **Observed Flow** options in the **Source/Sink/BC's** list. If you have more than one MODAEM model in your project, you will also need to select which model should be linked to the MODFLOW model using the **MODAEM models** combo box at the bottom of the *Coverage Setup* dialog.
3. Mark the boundaries (or at least the upstream and downstream boundaries) of the MODFLOW conceptual model as **MODAEM Head boundaries**.

At this point, whenever the ***Map->MODFLOW*** command is executed, GMS will automatically launch the MODAEM model and calculate a head value for each grid cell coinciding with the MODAEM Head boundary.

Furthermore, a flow value is computed for the boundary using MODAEM and assigned to the MODFLOW boundary as an observed head. This makes it possible to monitor the flow budget across the boundary to ensure that the changes made to the local scale model (insertion of remedial wells, etc.) do not violate the flow conditions inherited from the regional scale model.

MODAEM Output File

When MODAEM is executed, it generates an HTML formatted text output file. If the execution is successfully completed, an icon will appear under the corresponding MODAEM conceptual model in the Data Tree representing the output file. Double-clicking on this icon loads the output file into the default web browser.

MODAEM Links

- MODAEM License Agreement
- MODAEM Display Options

MODAEM License Agreement

GNU GENERAL PUBLIC LICENSE

Version 2, June 1991

59 Temple Place, Suite 330, Boston, MA 02111-1307 USA

Everyone is permitted to copy and distribute verbatim copies

of this license document, but changing it is not allowed.

Preamble

The licenses for most software are designed to take away your

freedom to share and change it. By contrast, the GNU General Public

License is intended to guarantee your freedom to share and change free

software--to make sure the software is free for all its users. This

General Public License applies to most of the Free Software

Foundation's software and to any other program whose authors commit to

using it. (Some other Free Software Foundation software is covered by

the GNU Library General Public License instead.) You can apply it to

your programs, too.

When we speak of free software, we are referring to freedom, not

price. Our General Public Licenses are designed to make sure that you

have the freedom to distribute copies of free software (and charge for

this service if you wish), that you receive source code or can get it

if you want it, that you can change the software or use pieces of it

in new free programs; and that you know you can do these things.

To protect your rights, we need to make restrictions that forbid

anyone to deny you these rights or to ask you to surrender the rights.

These restrictions translate to certain responsibilities for you if you distribute copies of the software, or if you modify it.

For example, if you distribute copies of such a program, whether gratis or for a fee, you must give the recipients all the rights that you have. You must make sure that they, too, receive or can get the source code. And you must show them these terms so they know their rights.

We protect your rights with two steps: (1) copyright the software, and (2) offer you this license which gives you legal permission to copy, distribute and/or modify the software.

Also, for each author's protection and ours, we want to make certain that everyone understands that there is no warranty for this free software. If the software is modified by someone else and passed on, we want its recipients to know that what they have is not the original, so that any problems introduced by others will not reflect on the original authors' reputations.

Finally, any free program is threatened constantly by software patents. We wish to avoid the danger that redistributors of a free program will individually obtain patent licenses, in effect making the program proprietary. To prevent this, we have made it clear that any patent must be licensed for everyone's free use or not licensed at all.

The precise terms and conditions for copying, distribution and modification follow.

GNU GENERAL PUBLIC LICENSE

TERMS AND CONDITIONS FOR COPYING, DISTRIBUTION AND MODIFICATION

0. This License applies to any program or other work which contains a notice placed by the copyright holder saying it may be distributed under the terms of this General Public License. The "Program", below, refers to any such program or work, and a "work based on the Program" means either the Program or any derivative work under copyright law: that is to say, a work containing the Program or a portion of it, either verbatim or with modifications and/or translated into another language. (Hereinafter, translation is included without limitation in the term "modification".) Each licensee is addressed as "you".

Activities other than copying, distribution and modification are not covered by this License; they are outside its scope. The act of running the Program is not restricted, and the output from the Program is covered only if its contents constitute a work based on the Program (independent of having been made by running the Program).

Whether that is true depends on what the Program does.

1. You may copy and distribute verbatim copies of the Program's source code as you receive it, in any medium, provided that you conspicuously and appropriately publish on each copy an appropriate copyright notice and disclaimer of warranty; keep intact all the notices that refer to this License and to the absence of any warranty; and give any other recipients of the Program a copy of this License along with the Program.

You may charge a fee for the physical act of transferring a copy, and you may at your option offer warranty protection in exchange for a fee.

2. You may modify your copy or copies of the Program or any portion of it, thus forming a work based on the Program, and copy and distribute such modifications or work under the terms of Section 1 above, provided that you also meet all of these conditions:

a) You must cause the modified files to carry prominent notices stating that you changed the files and the date of any change.

b) You must cause any work that you distribute or publish, that in whole or in part contains or is derived from the Program or any part thereof, to be licensed as a whole at no charge to all third parties under the terms of this License.

c) If the modified program normally reads commands interactively when run, you must cause it, when started running for such interactive use in the most ordinary way, to print or display an announcement including an appropriate copyright notice and a notice that there is no warranty (or else, saying that you provide a warranty) and that users may redistribute the program under these conditions, and telling the user how to view a copy of this License. (Exception: if the Program itself is interactive but does not normally print such an announcement, your work based on the Program is not required to print an announcement.)

These requirements apply to the modified work as a whole. If identifiable sections of that work are not derived from the Program, and can be reasonably considered independent and separate works in themselves, then this License, and its terms, do not apply to those sections when you distribute them as separate works. But when you distribute the same sections as part of a whole which is a work based on the Program, the distribution of the whole must be on the terms of this License, whose permissions for other licensees extend to the entire whole, and thus to each and every part regardless of who wrote it.

Thus, it is not the intent of this section to claim rights or contest
your rights to work written entirely by you; rather, the intent is to
exercise the right to control the distribution of derivative or
collective works based on the Program.
In addition, mere aggregation of another work not based on the Program
with the Program (or with a work based on the Program) on a volume of
a storage or distribution medium does not bring the other work under
the scope of this License.
3. You may copy and distribute the Program (or a work based on it,
under Section 2) in object code or executable form under the terms of
Sections 1 and 2 above provided that you also do one of the following:
a) Accompany it with the complete corresponding machine-readable
source code, which must be distributed under the terms of Sections
1 and 2 above on a medium customarily used for software interchange; or,
b) Accompany it with a written offer, valid for at least three
years, to give any third party, for a charge no more than your
cost of physically performing source distribution, a complete
machine-readable copy of the corresponding source code, to be
distributed under the terms of Sections 1 and 2 above on a medium
customarily used for software interchange; or,
c) Accompany it with the information you received as to the offer
to distribute corresponding source code. (This alternative is
allowed only for noncommercial distribution and only if you
received the program in object code or executable form with such
an offer, in accord with Subsection b above.)
The source code for a work means the preferred form of the work for
making modifications to it. For an executable work, complete source
code means all the source code for all modules it contains, plus any
associated interface definition files, plus the scripts used to
control compilation and installation of the executable. However, as a
special exception, the source code distributed need not include
anything that is normally distributed (in either source or binary
form) with the major components (compiler, kernel, and so on) of the
operating system on which the executable runs, unless that component
itself accompanies the executable.
If distribution of executable or object code is made by offering
access to copy from a designated place, then offering equivalent
access to copy the source code from the same place counts as
distribution of the source code, even though third parties are not

compelled to copy the source along with the object code.

4. You may not copy, modify, sublicense, or distribute the Program except as expressly provided under this License. Any attempt otherwise to copy, modify, sublicense or distribute the Program is void, and will automatically terminate your rights under this License. However, parties who have received copies, or rights, from you under this License will not have their licenses terminated so long as such parties remain in full compliance.

5. You are not required to accept this License, since you have not signed it. However, nothing else grants you permission to modify or distribute the Program or its derivative works. These actions are prohibited by law if you do not accept this License. Therefore, by modifying or distributing the Program (or any work based on the Program), you indicate your acceptance of this License to do so, and all its terms and conditions for copying, distributing or modifying the Program or works based on it.

6. Each time you redistribute the Program (or any work based on the Program), the recipient automatically receives a license from the original licensor to copy, distribute or modify the Program subject to these terms and conditions. You may not impose any further restrictions on the recipients' exercise of the rights granted herein. You are not responsible for enforcing compliance by third parties to this License.

7. If, as a consequence of a court judgment or allegation of patent infringement or for any other reason (not limited to patent issues), conditions are imposed on you (whether by court order, agreement or otherwise) that contradict the conditions of this License, they do not excuse you from the conditions of this License. If you cannot distribute so as to satisfy simultaneously your obligations under this License and any other pertinent obligations, then as a consequence you may not distribute the Program at all. For example, if a patent license would not permit royalty-free redistribution of the Program by all those who receive copies directly or indirectly through you, then the only way you could satisfy both it and this License would be to refrain entirely from distribution of the Program.

If any portion of this section is held invalid or unenforceable under any particular circumstance, the balance of the section is intended to apply and the section as a whole is intended to apply in other circumstances.

It is not the purpose of this section to induce you to infringe any patents or other property right claims or to contest validity of any such claims; this section has the sole purpose of protecting the integrity of the free software distribution system, which is implemented by public license practices. Many people have made generous contributions to the wide range of software distributed through that system in reliance on consistent application of that system; it is up to the author/donor to decide if he or she is willing to distribute software through any other system and a licensee cannot impose that choice.

This section is intended to make thoroughly clear what is believed to be a consequence of the rest of this License.

8. If the distribution and/or use of the Program is restricted in certain countries either by patents or by copyrighted interfaces, the original copyright holder who places the Program under this License may add an explicit geographical distribution limitation excluding those countries, so that distribution is permitted only in or among countries not thus excluded. In such case, this License incorporates the limitation as if written in the body of this License.

9. The Free Software Foundation may publish revised and/or new versions of the General Public License from time to time. Such new versions will be similar in spirit to the present version, but may differ in detail to address new problems or concerns.

Each version is given a distinguishing version number. If the Program specifies a version number of this License which applies to it and "any later version", you have the option of following the terms and conditions either of that version or of any later version published by the Free Software Foundation. If the Program does not specify a version number of this License, you may choose any version ever published by the Free Software Foundation.

10. If you wish to incorporate parts of the Program into other free programs whose distribution conditions are different, write to the author to ask for permission. For software which is copyrighted by the Free Software Foundation, write to the Free Software Foundation; we sometimes make exceptions for this. Our decision will be guided by the two goals of preserving the free status of all derivatives of our free software and of promoting the sharing and reuse of software generally.

NO WARRANTY

11. BECAUSE THE PROGRAM IS LICENSED FREE OF CHARGE, THERE IS NO WARRANTY

FOR THE PROGRAM, TO THE EXTENT PERMITTED BY APPLICABLE LAW. EXCEPT WHEN OTHERWISE STATED IN WRITING THE COPYRIGHT HOLDERS AND/OR OTHER PARTIES PROVIDE THE PROGRAM "AS IS" WITHOUT WARRANTY OF ANY KIND, EITHER EXPRESSED OR IMPLIED, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE. THE ENTIRE RISK AS TO THE QUALITY AND PERFORMANCE OF THE PROGRAM IS WITH YOU. SHOULD THE PROGRAM PROVE DEFECTIVE, YOU ASSUME THE COST OF ALL NECESSARY SERVICING, REPAIR OR CORRECTION.

12. IN NO EVENT UNLESS REQUIRED BY APPLICABLE LAW OR AGREED TO IN WRITING WILL ANY COPYRIGHT HOLDER, OR ANY OTHER PARTY WHO MAY MODIFY AND/OR REDISTRIBUTE THE PROGRAM AS PERMITTED ABOVE, BE LIABLE TO YOU FOR DAMAGES, INCLUDING ANY GENERAL, SPECIAL, INCIDENTAL OR CONSEQUENTIAL DAMAGES ARISING OUT OF THE USE OR INABILITY TO USE THE PROGRAM (INCLUDING BUT NOT LIMITED TO LOSS OF DATA OR DATA BEING RENDERED INACCURATE OR LOSSES SUSTAINED BY YOU OR THIRD PARTIES OR A FAILURE OF THE PROGRAM TO OPERATE WITH ANY OTHER PROGRAMS), EVEN IF SUCH HOLDER OR OTHER PARTY HAS BEEN ADVISED OF THE POSSIBILITY OF SUCH DAMAGES.

END OF TERMS AND CONDITIONS

How to Apply These Terms to Your New Programs

If you develop a new program, and you want it to be of the greatest possible use to the public, the best way to achieve this is to make it free software which everyone can redistribute and change under these terms.

To do so, attach the following notices to the program. It is safest to attach them to the start of each source file to most effectively convey the exclusion of warranty; and each file should have at least the "copyright" line and a pointer to where the full notice is found.

}}--> This is free software, and you are welcome to redistribute it
under certain conditions; type `show c' for details.

The hypothetical commands `show w' and `show c' should show the appropriate parts of the General Public License. Of course, the commands you use may be called something other than `show w' and `show c'; they could even be mouse-clicks or menu items--whatever suits your program.

You should also get your employer (if you work as a programmer) or your school, if any, to sign a "copyright disclaimer" for the program, if necessary. Here is a sample; alter the names:

Yoyodyne, Inc., hereby disclaims all copyright interest in the program `Gnomovision' (which makes passes at compilers) written by James Hacker.

, 1 April 1989

Ty Coon, President of Vice

This General Public License does not permit incorporating your program into proprietary programs. If your program is a subroutine library, you may consider it more useful to permit linking proprietary applications with the library. If this is what you want to do, use the GNU Library General Public License instead of this License.

MODAEM Display Options

The properties of all MODAEM properties that GMS displays on the screen can be controlled through the MODAEM tab of the *Display Options* dialog. This dialog is opened by right clicking on the  Map Data entry in the Project Explorer, selecting the Display Options command, and then selecting the MODAEM tab. This tab is only visible when there is a MODAEM simulation. It can also be accessed from the from the Display menu, the *MODAEM* menu, or the  Display Options macro. The following table describes the display options available for the MODAEM model.

Display Option	Description
Contours	Whenever MODAEM is executed, the head values are computed at the corners of a background grid. These head values can then be contoured. Most of the objects supported by GMS can be contoured by turning on the Contour in the *Display Options* dialog. When an object is contoured, the values associated with the active data set for the object are used to generate the contours.
Map elevations	If the Map Elevations option is selected in the *MODAEM Display Options* dialog, the head values are mapped to elevations (z values) of the background grid and the contours are displayed on the resulting warped grid in oblique view. This makes it possible to see a 3D view of the computed water table surface.
Background mesh	Controls the displays of a background grid. The density of the background grid can be adjusted using the Mesh density factor edit field. The background grid is always adjusted to fit the area defined by the boundary polygon or the GMS graphics window. If you zoom in to look at a local area of the model and select the **F5** button, the background grid is rebuilt to fit the current viewing area. In this manner, one can view the solution at any desired level of detail.
Pathlines	The pathlines can be toggled on and off, and the pathline style and color can be adjusted. The pathline color can be set to the default color, or the color corresponding to the starting or ending zone codes of the pathlines. If the Pathlines option is turned on for one or more MODAEM wells, a set of pathlines are automatically computed by MODAEM and displayed when the solution is updated. For wells, pathlines are always computed backwards in time. The display options associated with the pathlines (max tracking time, direction arrows, etc.) can be controlled using the *MODAEM Display Options* dialog. Particles may also be created at user-specified points in the aquifer, including a starting elevation. GMS will pass these points to MODAEM for forward tracing. Currently, GMS does not provide a way to trace these particles backwards in time.
Direction arrows	Direction arrows can be displayed along the pathlines. The size of the arrow heads can be set by specifying the Length in pixels. The arrows are displayed along the pathline at an interval corresponding to the Length specified.
Dry wells	Controls the display of wells that have gone dry during the MODAEM simulation run. They symbol, symbol size, and symbol color can be adjusted by clicking on the button to the left of the toggle.
Reference point	Controls the display of reference points. They symbol, symbol size, and symbol color can be adjusted by clicking on the button to the left of the toggle.

MODAEM Commands

Menu Command	Description
Global Options...	
Display Options...	
Solve	
Pathlines -> Arcs	
Contours -> Arcs	

6.3. MODFLOW

MODFLOW

MODFLOW	
Model Info	
Model type	3D, cell-centered finite-difference, saturated flow model, steady state and transient analysis
Supported versions	MODFLOW-88*, MODFLOW-96*, MODFLOW-2000, MODFLOW-2005, MODFLOW-NWT, MODFLOW-LGR** * import only ** coming soon
Developer	USGS, [1]
Documentation	MF2K Flow Process [2] MF2005 Flow Process [3] MF NWT [4] MF-LGR [5] MF-LGR-mult [6] MF-LGR-SFR [7]
Tutorials	MODFLOW Tutorials
Packages	**Flow:** BCF6, HUF, LPF, UPW **Solvers:** DE4, GMG, NWT, PCG2, SAMG, SIP, SOR **Other:** BAS6, CHD1, DRN1, DRT1, EVT1, ETS1, GAGE, GHB1, HFB1, HUF, LAK3, MNW1, MNW2, OUT1, RCH1, RIV1, SFR2, STR1, SUB1, WEL1, UZF1

GMS includes a comprehensive graphical interface to the groundwater model MODFLOW. MODFLOW is a 3D, cell-centered, finite difference, saturated flow model developed by the United States Geological Survey (McDonald & Harbaugh, 1988). MODFLOW can perform both steady state and transient analyses and has a wide variety of boundary conditions and input options.

GMS supports MODFLOW as a pre- and post-processor. The input data for MODFLOW are generated by GMS and saved to a set of files. These files are read by MODFLOW when MODFLOW is launched from the *GMS* menu. The output from MODFLOW is then imported to GMS for post-processing.

A special version of MODFLOW is distributed with GMS. This version of MODFLOW is the same as the version distributed by the USGS except for a few minor changes primarily related to file input including reading input data from HDF5 files. These changes are clearly marked in the code. For more information see MODFLOW with HDF5.

To learn more about using MODFLOW in GMS, please refer to the available tutorials.

More information about MODFLOW is available from the USGS [1].

MODFLOW Versions

GMS supports (or will soon) all standard MODFLOW versions:

- MODFLOW-88 (import only)
- MODFLOW-96 (import only)
- MODFLOW-2000
- MODFLOW-2005
- MODFLOW-NWT
- MODFLOW-LGR (coming soon)
- MODFLOW-USG (under development)

Pre-Processing

- Importing MODFLOW Files
- Building a MODFLOW Model
- Saving a MODFLOW Simulation
- Parameters
- Stochastic Modeling with MODFLOW
- Interpolate to MODFLOW Layers
- Packages Supported in GMS
- Unsupported MODFLOW Features

Post-Processing

- MODFLOW Display Options
- MODFLOW Post Processing Viewing Options
- Reading a MODFLOW Simulation

MODFLOW Documentation

MODFLOW 88I [8]
MODFLOW 88II [9]
MODFLOW 96I [10]
MODFLOW 96II [11]
MF2K Calibration [12]
MF2K Flow Process [2]
MF2K HUF [13]
MF2K LMG [14]
MF2K LMT [15]
MF2K obssenspeprocess [16]
MF2005 Flow Process [3]
MF NWT [4]

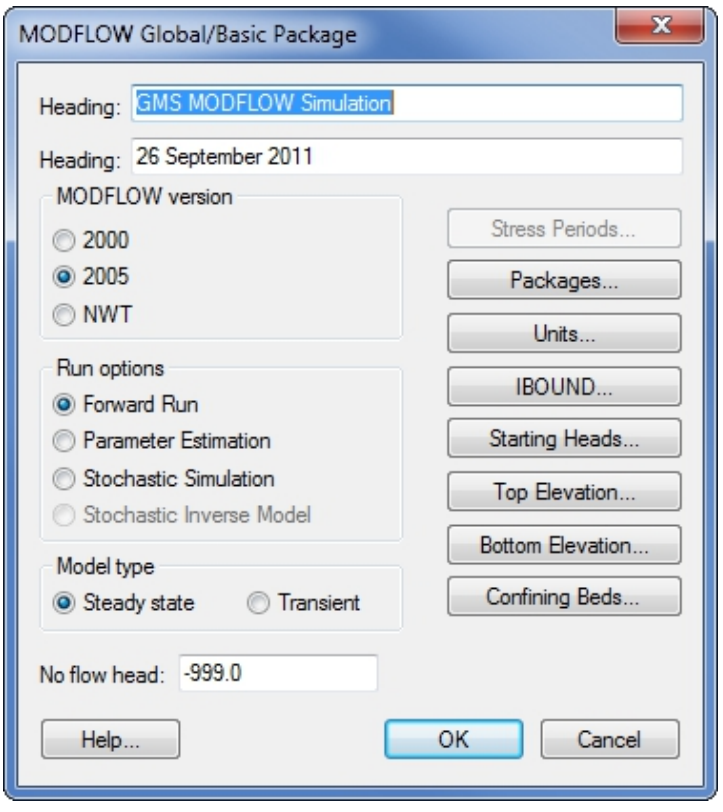
References

[1] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/
[2] http://gmsdocs.aquaveo.com/mf2k_flowprocess.pdf
[3] http://gmsdocs.aquaveo.com/mf2005_flowprocess.pdf
[4] http://gmsdocs.aquaveo.com/MF_NWT.pdf
[5] http://gmsdocs.aquaveo.com/MF-LGR.pdf
[6] http://gmsdocs.aquaveo.com/MF-LGR-mult.pdf
[7] http://gmsdocs.aquaveo.com/MF-LGR-SFR.pdf
[8] http://gmsdocs.aquaveo.com/modflow88I.pdf
[9] http://gmsdocs.aquaveo.com/modflow88II.pdf
[10] http://gmsdocs.aquaveo.com/modflow96I.pdf
[11] http://gmsdocs.aquaveo.com/modflow96II.pdf
[12] http://gmsdocs.aquaveo.com/mf2k_calibration.pdf
[13] http://gmsdocs.aquaveo.com/mf2k_huf.pdf
[14] http://gmsdocs.aquaveo.com/mf2k_lmg.pdf
[15] http://gmsdocs.aquaveo.com/mf2k_lmt.pdf
[16] http://gmsdocs.aquaveo.com/mf2k_obssenspeprocess.pdf

MODFLOW-2005

Choosing MODFLOW 2000 or MODFLOW 2005

Choosing to use MODFLOW 2000 or MODFLOW 2005 is done in the MODFLOW Global Options Dialog. At any time you can switch from one to the other.



MODFLOW Global Option Dialog

Changes in MODFLOW 2005

The following list shows changes in MODFLOW 2005 from MODFLOW 2000.

1. **SOR1 Solver**

- MODFLOW 2005 no longer supports the SOR1 Solver.

2. **PCG2 Solver**

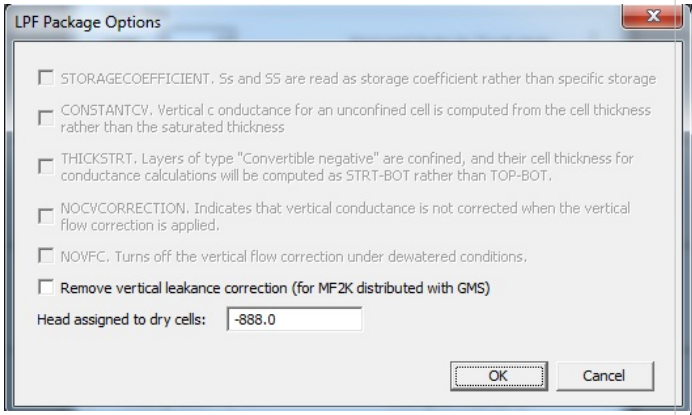
- MODFLOW 2005 replaces the DAMP variable with DAMPPCG and DAMPPCGT variables [1]. These two new variables allow different damping factors to be applied separately to steady-state and transient stress periods.

3. **UZF Package**

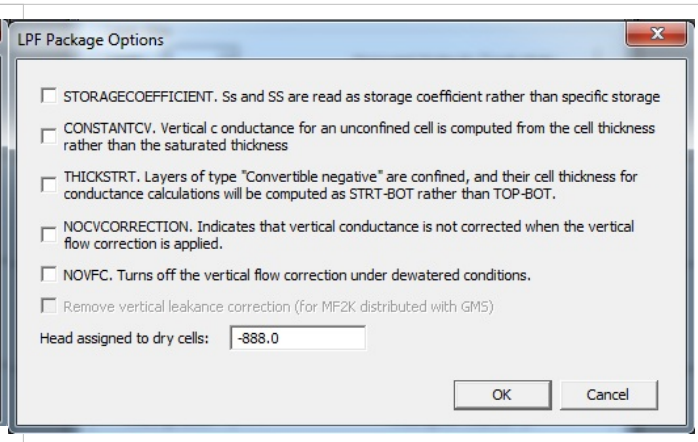
- MODFLOW 2005 added support for the Unsaturated Zone Flow (UZF) package.

4. **LPF package**

- MODFLOW 2005 provides more options for the LPF Package. Pictures below show the LPF package options supported in MODFLOW 2000 vs MODFLOW 2005.



MODFLOW 2000 LPF Package Options



MODFLOW 2005 LPF Package Options

5. **PES and PEST**

- PES is not available in MODFLOW 2005. Automated calibration in GMS is handled using PEST.

References

[1] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/index.html?pcg.htm

MODFLOW Commands

Menu Command	Description
New Simulation...	Creates a new MODFLOW simulation and brings up the *Global Options/Basic Package* dialog. If a simulation exists then the current one will be deleted and a new one will be made.
Delete Simulation...	Deletes the current MODFLOW simulation.
Check Simulation...	Brings up the *Model Checker* dialog. This generates a list of possible errors and warning messages in the top scrolling window.
Run MODFLOW...	Initiates the MODFLOW executable. GMS will ask if you would like to save your work before running the executable.
Read Solution...	Opens a window for the user to search for a previous MODFLOW solution.
Flow Budget...	Shows the model's flow budget as one zone (default) or multiple user defined zones.
Export Native MF2K text...	Creates native MODFLOW files from existing GMS MODFLOW-with-hdf5 files.
Display Options...	
Sources/Sinks...	
Toggle Barrier	Creates a "no flow boundary" between two adjacent selected cells.
Cell Properties...	
IFACE...	
ITOP...	
Global Options...	Opens the Global/Basic Package dialog to set up a MODFLOW simulation.

LPF Package...	Opens the flow dialog to insert hydrologic parameters. (May not be LPF)
PCG2 Package...	Opens the solver dialog for the selected solver. (May not be PCG2)
Source/Sink Packages >	
Well (WEL) Package...	
Multi-Node Well (MNW) Package...	
River (RIV) Package...	
Lake (LAK) Package...	
Drain (DRN) Package...	
Drain Return (DRT) Package...	
General Head (GHB) Package...	
Recharge (RCH) Package...	
Evapotranspiration (EVT) Package...	
Evapotranspiration Segment (ETS) Package...	
Stream (STR) Package...	
Stream (SFR2) Package...	
Time Var. Head (CHD) Package...	
Unsaturated Zone (UZF) Package...	
Output Control...	Opens an output dialog for the user to chose what comes out of a MODFLOW run.
HFB Package...	
Convergence Options...	
Parameters...	
Obervations...	
Parameter Estimation...	
Stochastic...	

6.3.1. MODFLOW Packages

MODFLOW Packages Supported in GMS

MODFLOW is divided into a series of components called "packages." Each package performs a specific task. The input for each package is generally contained in a separate file. The MODFLOW packages supported by GMS are listed in the following tables.

The MODFLOW packages to be used in the MODFLOW simulation are specified in the Packages dialog. This dialog is accessed in the *Global Options\Basic Package* dialog. Some of the packages are always required for a simulation and some are optional. One of the flow model packages and one of the solver packages must be selected. Each of the boundary condition/source/sink packages is optional.

For any package not currently supported in GMS, the file associated with that package will be ignored when the model is imported. However, GMS keeps track of unsupported packages it encounters when reading the name file and, when the project is saved, GMS lists the unsupported packages in the name file and copies the unsupported package files from the old directory to the new directory.

Global Options & Output

Abrev Name	Package/File Name	USGS	Description	Always Req'd?	Extension
MFN	Name file	[1]	The MODFLOW name file. GMS uses "mfn" as the extension.	Yes	*.mfn
BAS6	Basic Package	[2]	Used to specify the grid dimensions, the computational time steps, and an array identifying which packages are to be used.	Yes	*.bas
DIS	Discretization File	[3]	The Discretization File is used to specify certain data used in all models. These include, the number of rows, columns and layers, the cell sizes, the presence of Quasi-3D confining beds, the time discretization.	Yes	*.dis
OUT1	Output Control	[4]	Controls what information is to be output from MODFLOW and when it is to be output.	No	*.oc

Flow Packages

Interfaces to four different flow packages are provided in GMS: the block centered flow (BCF), the layer property flow (LPF), the hydrogeologic unit flow (HUF), and the upstream weighting (UPW) packages. One of these four packages must be selected in the Packages dialog.

Abrev Name	Package Name	USGS	Description	Always Req'd?	Extension
BCF6	Block Centered Flow Package	[5]	Performs the cell by cell flow calculations. The input to this package includes layer types and cell attributes such as storage coefficients and transmissivity. Parameters for sensitivity analysis or parameter estimation are NOT supported.	Yes[1]	*.bcf
LPF	Layer Property Flow Package	[6]	Performs the cell by cell flow calculations. The input to this package includes layer types and cell attributes such as storage coefficients and transmissivity.	Yes[1]	*.lpf
UPW	Upstream Weighting Flow Package	[7]	Based on the LPF package. Modified to provide a linear formulation that can be used with the NWT solver.	Yes[1]	*.upw
HUF	Hydrogeologic Unit Flow Package	[8]	Defines the model stratigraphy in a grid independent fashion (in the vertical direction).	Yes[1]	*.huf

[1] One of the flow packages must be used.

Solver Packages

Abrev Name	Package Name	USGS	Description	Always Req'd?	Extension
GMG	Geometric Multi-Grid	[9]	The Geometric Multigrid Solver is used to solve the finite difference equations in each step of a MODFLOW stress period.	Yes[1]	*.gmg
SIP	Strongly Implicit Procedure	[10]	The Strongly Implicit Procedure package is used to solve the finite difference equations in each step of a MODFLOW stress period.	Yes[1]	*.sip
PCG2	Preconditioned Conjugate Gradient Method	[11]	The Preconditioned Conjugate-Gradient package is used to solve the finite difference equations in each step of a MODFLOW stress period.	Yes[1]	*.pcg
PCGN	Preconditioned Conjugate Gradient Solver with Improved Nonlinear Control	[12]	The Preconditioned Conjugate-Gradient package is used to solve the finite difference equations in each step of a MODFLOW stress period.	Yes[1]	*.pcgn
SOR	Slice-Successive Overrelaxation Method	[13]	The Slice-Successive Overrelaxation package is used to solve the finite difference equations in each step of a MODFLOW stress period.	Yes[1]	*.sor
SAMG or LINK-AMG	Algebraic MultiGrid for Systems Solver	[14]	The Link-AMG package is used to solve the finite difference equations in each step of a MODFLOW stress period.	Yes[1]	*.lmg
DE4	Direct Solver	[15]	The DE4 package is used to solve the finite difference equations in each step of a MODFLOW stress period.	Yes[1]	*.de4
NWT	Newton Solver	[16]	The NWT package is used to solve the finite difference equations in each step of a MODFLOW-NWT stress period.	Yes[1]	*.nwt

[1] One of these solvers must be selected in the Packages dialog.

Once a solver has been selected, the appropriate solver package dialog can be accessed through one of the solver commands (LMG, SIP, PCG2, or SSOR) in the *MODFLOW* menu. The default values shown in each dialog are typically adequate.

For more information on Solver Packages visit: http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/index.html

Optional Packages

Abrev Name	Package Name	USGS	Description	Always Req'd?	Extension
BFH	Boundary Flow and Head Package	[17]	Used with MODFLOW-LGR to use coupled flows and heads when running parent or child model independently.	No	*.bfh_hed, *.bfh_flw
DRN1	Drain Package	[18]	Simulates drain type boundary conditions.	No	*.drn
DRT1	Drain Return Package	[19]	Simulates drain return type boundary conditions.	No	*.drt
EVT1	Evapotranspiration Package	[20]	Simulates the effect of evapotranspiration in the vadose zone.	No	*.evt
ETS1	Evapotranspiration Segments Package	[21]	"allows simulation of evapotranspiration with a user-defined relation between evapotranspiration rate and hydraulic head."[22]	No	*.ets
GAGE	Gage Package	[23]	Allows SFR and lake gaging stations. Gaging station prints time series values for gage location.	No	*.gag
GHB1	General Head Boundary Package	[24]	Simulates a general purpose head-dependent source/sink. Commonly used to simulate lakes.	No	*.ghb
HFB1	Horizontal Flow Barrier Package	[25]	Simulates the effect of horizontal flow barriers such as sheet piles and slurry trenches.	No	*.hfb
LAK3	Lake Package	[26]	A more sophisticated alternative to the typical approach of using the General head package to simulate the effect of lakes and reservoirs. Computes the stage based on the water budget unlike the GHB.	No	*.lak
MNW1	Multi-Node Well 1 Package	[27]	older revision of MNW package used to simulate wells that extend over more than one cell.	No	*.mnw
MNW2	Multi-Node Well 2 Package	[28]	updated revision of MNW1 package used to simulate wells that extend over more than one cell.	No	*.mnw2
RCH1	Recharge Package	[29]	Simulates recharge to the groundwater from precipitation.	No	*.rch
RIV1	River Package	[30]	Simulates river type boundary conditions.	No	*.riv
SFR2	Streamflow-Routing Package	[31]	Simulates the exchange of water between the aquifer and surficial streams. Includes routing and automatic computation of stage. Parameters for sensitivity analysis or parameter estimation are NOT supported.	No	*.sfr
STR1	Stream-Routing Package	[32]	Simulates the exchange of water between the aquifer and surficial streams. Includes routing and automatic computation of stage. Parameters for sensitivity analysis or parameter estimation are NOT supported.	No	*.str
CHD1	Time Variant Specified Head Package	[33]	Simulates specified head boundary conditions where the head is allowed to vary with time.	No	*.chd
SUB1	Subsidence Package	[34]	Simulates simulates aquifer compaction and land subsidence.	No	*.sub
WEL1	Well Package	[35]	Simulates injection/extraction wells.	No	*.wel
UZF1	Unsaturated-Zone Flow Package	[36]	Simulate percolation of water through the unsaturated zone.	No	*.uzf

Other Files

Other files that GMS reads and writes with MODFLOW simulations.

File Name	Description	Extension
MFS	MODFLOW "Super" file, created by GMS to keep track of extra information GMS needs.	*.mfs
MFS	MODFLOW World file, created by GMS to keep track of the geographic location of a MODFLOW model.	*.mfw
PRJ	Projection file in ArcGIS well-known text [37] format specifying a geographic coordinate system.	*.prj
H5	An HDF5 formatted file containing array and list data referenced from other package files. See MODFLOW_with_HDF5 for more information	*.h5
ASP	A file used with a special version of MODFLOW modified to use PEST.	*.asp
PARAM	Extra information about the parameters used by GMS and our modified version of MODFLOW.	*.param
M2P	Used by MF2PEST.EXE program.	*.m2p

Output Files

Standard Extensions for OUTPUT files.

Package	Extension
	*.ccf
Drawdown	*.drw
Global	*.glo
Head	*.hed
Output	*.out

If a fort.# file occurs the MODFLOW file was written to the given unit number.

If a file has an underscore (*_...) followed by an extension refer to pages 29 and 30 of the MODFLOW Documentation linked here:MF2K Obs-Sen-Pes [38]

Notes

[1] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/name_file.htm
[2] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/bas6.htm
[3] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/dis.htm
[4] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/oc.htm
[5] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/bcf.htm
[6] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/lpf.htm
[7] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/upw_upstream_weighting_package.htm
[8] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/huf2.htm
[9] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/gmg.htm
[10] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/sip.htm
[11] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/pcg.htm
[12] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/pcgn.htm
[13] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/sor.htm
[14] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/lmg.htm
[15] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/de4.htm
[16] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/nwt_newton_solver.htm
[17] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/bfh___boundary_flow_and_head_p.htm
[18] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/drn.htm
[19] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/drt.htm

[20] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/evt.htm
[21] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/ets.htm
[23] http://water.usgs.gov/nrp/gwsoftware/modflow2000/Guide/index.html?gage.htm
[24] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/ghb.htm
[25] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/hfb6.htm
[26] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/lak.htm
[27] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/mnw.htm
[28] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/mnw2.htm
[29] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/rch.htm
[30] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/riv.htm
[31] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/sfr.htm
[32] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/str.htm
[33] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/chd.htm
[34] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/sub.htm
[35] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/wel.htm
[36] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/index.html?uzf_unsaturated_zone_flow_pack.htm
[37] http://en.wikipedia.org/wiki/Well-known_text
[38] http://pubftp.ems-i.com/download/GMS/GMS%206.5/models/mf2k_obssenspeprocess.pdf

BCF Package

NOTE: The observation, sensitivity, and parameter estimation processes do not support the BCF package.

Once the data in the Global Options/Basic Package are initialized, the data for the flow package can be defined. The BCF package is one of three flow packages that can be used. The BCF package computes the conductance between each of the grid cells and sets up the finite difference equations for the cell to cell flow. It also computes the terms that determine the rate of movement of water to and from storage. The *BCF Package* dialog is accessed through the ***BCF Package*** command in the *MODFLOW* menu.

Data Required

Data arrays required for a particular layer are dependent on the layer type. The layer arrays required for each layer type are shown in the following table. The leakance array is not required for the bottom layer and the storage coefficients are only required for transient simulations.

Layer Type	Required Arrays
Confined (LAYCON=0)	Transmissivity, Leakance, Primary Storage Coefficient (Storativity)
Unconfined (LAYCON=1)	Bottom Elevation, Hydraulic Conductivity, Leakance, Primary Storage Coefficient (Specific yield)
Confined/Unconfined (LAYCON=2)	Top Elevation, Transmissivity, Leakance, Primary Storage Coefficient (Storativity), Secondary Storage Coefficient (Specific yield)
Confined/Unconfined (LAYCON=3)	Top Elevation, Bottom Elevation, Hydraulic Conductivity, Leakance, Primary Storage Coefficient (Storativity), Secondary Storage Coefficient (Specific yield)

Each of the required input arrays must be entered by the user for each layer. Some of the layer arrays can be directly entered. However, some are dependent on the layer geometry. For example, leakance is a function of the layer thickness and the vertical hydraulic conductivity. The transmissivity is equal to the horizontal hydraulic conductivity multiplied by the layer thickness.

The BCF Package can be used for simple models with a single layer for multiple layers with simple stratigraphy. In such cases, many of the parameters are constant for an entire layer and can be entered directly. For more complex models, the following steps can be taken to prepare the input arrays (or the user can use the LPF package):

1. Import a set of scatter points defining the elevations of the stratigraphic horizons.

2. Interpolate the top and bottom elevations of each unit to a 2D grid which matches the 3D computational grid.
3. Compute the desired parameter arrays using the interpolated elevation arrays and the Data Calculator.
4. Copy the parameter arrays into the appropriate MODFLOW arrays in the *BCF Package* dialog.

Since this approach can be quite time-consuming, the LPF Package is recommended for most models.

Layer Data

The aquifer properties are entered in the layer data section.

Layer

The layer edit field is used to select the layer. The buttons on the right side of the dialog apply to the active layer only.

Layer Data Arrays

The six buttons on the right portion of the dialog represent layer data arrays such as elevations and hydraulic conductivity. Each of the six buttons brings up a dialog for entering an array of values. The dialog can be used to edit individual values, assign a constant value to the entire array, or to copy a data set generated by interpolating from a scatter point set to the array.

Not all of the data arrays need to be specified for each layer. Some arrays are only required for transient models. The required arrays depend on the layer type.

Layer data arrays can also be edited using other tools in GMS. The array values can be edited by selecting a set of cells and using the ***Cell Properties*** command. The values in the layer parameter arrays can be initialized using coverages of a conceptual model defined in the Map module. A set of tools for rapidly defining top and bottom elevations is provided (See Defining Layer Elevations). Layer data can also be assigned using material zones.

Layer Type

Each layer must be assigned a layer type (LAYCON). By default, the top layer is defined to be an unconfined layer and all other layers are initialized as confined. The data arrays required by a layer may be dependent on the layer type.

Interblock Transmissivity

The method used for computing interblock transmissivity is specified using the pull-down list in the middle right portion of the *BCF Package* dialog.

Anisotropy Factor

This edit field allows the user to adjust the anisotropy that should be used in the model. This value is defaulted to 1.0.

Head Assigned to Dry Cells

This edit field allows the user to adjust the default head value assigned to dry cells. This value is defaulted to -888.0 or -999.0.

Cell Rewetting Parameters

The controls related to rewetting cells in the lower left portion of the *BCF Package* dialog are only activated if the BCF2 or BCF3 package has been specified. If wetting of cells is to be allowed, a wetting factor, wetting iteration

interval, and wetting equation must be specified.

Storage coefficients

Name	Description	Units
Storativity	"the volume of water released from storage per unit decline in hydraulic head in the aquifer, per unit area of the aquifer"[1]	unitless
Specific Storage (Ss)	"the amount of water that a portion of an aquifer releases from storage, per unit mass or volume of aquifer, per unit change in hydraulic head"[1]	1/L
Specific Yield (Sy)	"also known as the drainable porosity, is a ratio, less than or equal to the effective porosity, indicating the volumetric fraction of the bulk aquifer volume that a given aquifer will yield when all the water is allowed to drain out of it under the forces of gravity"[1]	unitless

References

[1] http://en.wikipedia.org/wiki/Specific_storage

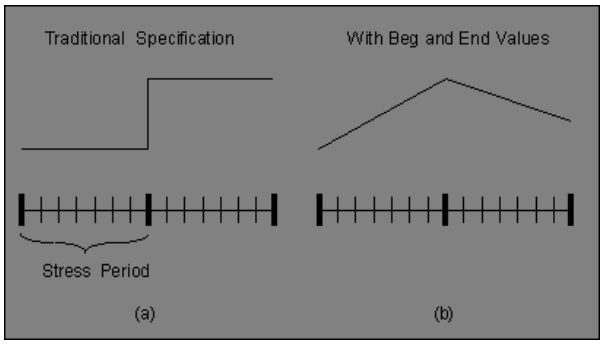
CHD Package

In the original version of MODFLOW, specified head boundaries are defined using a combination of the IBOUND array and the starting heads array. Since both of these arrays are static, boundaries where the head varies with time could not be simulated. To address this type of boundary, a new package called the Time Variant Specified Head (CHD) package has been developed.

NOTE: GMS does not support parameters for the Time Varient Specified Head (CHD) package.

Specifying Transient Head Values

Transient data are handled in a unique fashion with the CHD package. When transient values are assigned to the other stress packages, one value is assigned per stress period. The value represents the value at the beginning of the stress period. This results in a stair step definition of the time series as shown in part a of the following figure. With the CHD package, two values are assigned per stress period: a value at the beginning of the stress period and a value at the end of the stress period. This makes it possible to specify a piece-wise linear time series as shown in part b.



Specifying Transient Values Using (a) the Traditional Approach and (b) the Approach Used in the CHD Package.

Defining Time Variant Specified Head Boundaries

A time variant specified head boundary can be defined using a conceptual model in the Map module simply by using the Transient option when entering the head value in the Attributes dialog. When the specified head attribute is assigned to a polygon, the head is assigned uniformly over the entire polygon. When assigned to an arc, separate head values are applied to each of the nodes on the ends of the arc and the head is assumed to vary linearly between the nodes. When the attribute is assigned to a point, the head is assigned directly to the cell containing the point. For cell-by-cell editing, a selected set of cells can be designated as time variant specified head cells using the ***Point Sources/Sinks*** command described above. When the head vs. time values are entered using the XY Series Editor, two values (beginning and ending values) must be entered per stress period. Once a set of cells has been specified, the Time Variant Specified Head Package dialog can be used to view and edit the values assigned to the cells.

Stress Period

This field shows the current stress period and allows you to cycle through the stress periods and view the different head properties for those stress periods in the spreadsheet below.

Use Previous

Use this option on a stress period to use the values from the previous stress period for the current stress period. This option is unavailable for steady state models and the first stress period of transient models.

Spreadsheet

For cells where CHD type boundary conditions have been assigned, the starting and ending heads assigned to each cell are displayed in the spreadsheet portion at the lower part of the dialog. The spreadsheet can be used to edit the row, column, layer, starting head, and ending head values. For a transient simulation, the values displayed in the spreadsheet are for an individual stress period. The values associated with other stress periods can be edited by entering the number of the desired stress period in the stress period edit box in the center of the dialog. If the Use previous option is selected for a given stress period, the values from the previous stress period are used and the spreadsheet is dimmed.

Reset

This button restores all values in the dialog to their default values

DE4 Package

The DE4 package or Direct Solver is one of the solvers available for MODFLOW.

For more information on this solver see the USGS documentation here. [1]

References

[1] http://pubs.er.usgs.gov/usgspubs/ofr/ofr200092

DRN Package

The Drain package is used to simulate the effect of drains on an aquifer. Drains remove water from the aquifer as long as the water table is above the elevation of the drain. If the water table falls below the elevation of the drain, the drain has no effect. The rate of removal is proportional to the difference in elevation between the water table and the drain. The constant of proportionality is the conductance of the fill material surrounding the drain.

A set of selected cells can be specified as drains using the Point Sources/Sinks command in the MODFLOW menu or drains can be defined using the conceptual model approach in the map module. Drains are specified by assigning an elevation and a conductance to each cell at the location of each drain.

The drain attribute may be associated with points, arcs, or polygons. There are two parameters that are associated with a drain: elevation and conductance. Elevation may be specified as a constant value or transient series, or interpolated from an existing TIN. Conductance may be constant or vary with time.

When a polygon is defined as a drain, the elevation and conductance values (constant or time-varying) are applied uniformly over the entire polygon. When an arc is assigned to be a drain, the conductance is applied uniformly over the arc but separate elevation values are applied to each of the nodes on the ends of the arc and the elevation is assumed to vary linearly between the nodes. When a point is classified as a drain, the elevation and conductance values are assigned directly to the cell containing the point.

See also the Drain Return Package.

Stress Period

This field shows the current stress period and allows you to cycle through the stress periods and view the different river properties for those stress periods in the spreadsheet below.

Use Previous

Use this option on a stress period to use the drain values from the previous stress period for the current stress period. This option is unavailable for steady state models and the first stress period of transient models.

Spreadsheet

For cells where drain type boundary conditions have been assigned, the conductance, elevation, and conductance factor assigned to each cell are displayed in the spreadsheet portion at the lower part of the dialog. The spreadsheet can be used to edit the row, column, layer, conductance, and elevation values. For a transient simulation, the values displayed in the spreadsheet are for an individual stress period. The values associated with other stress periods can be edited by entering the number of the desired stress period in the stress period edit box in the center of the dialog. If the Use previous option is selected for a given stress period, the values from the previous stress period are used and the spreadsheet is dimmed. The conductance factor is used, and only appears in the spreadsheet, with DRN parameter estimation. When doing parameter estimation the value of drain conductance assigned to a particular drain

boundary condition will be the value of the drain parameter multiplied by the conductance factor. For more information on DRN parameters and conductance factors see the MODFLOW 2000 manual.

Display Cell IDs/IJK

The radio group at the bottom of the dialog allows the user to adjuster whether the cell ID or the cell i, j, k values are displayed for the cells containing the boundary condition/source/sink.

Delete All

The Delete All button deletes all of the data currently defined in the River package and restores the River package parameters to the default values.

DRT Package

The Drain Return Package (DRT) is very similar to the regular Drain Package (DRN). Drains remove water from the aquifer as long as the water table is above the elevation of the drain. With the DRT package, some percentage of that removed water can be reintroduced to the aquifer at a specified grid cell.

DRT boundary conditions can be added to selected cells using the ***Point Sources/Sinks*** command in the *MODFLOW* menu. DRT objects can also be defined using the conceptual model approach in the map module.

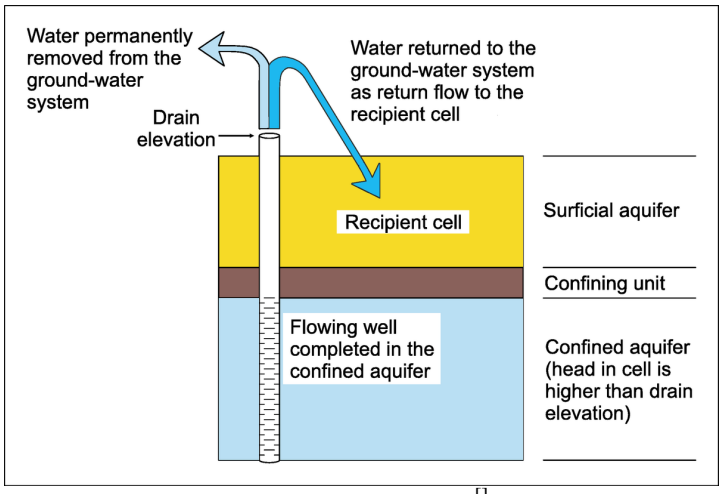


Illustration of DRT package[]

Conceptual model

Drains can be modeled using points, arcs and/or polygons in a conceptual model. The return cell cannot be specified in the conceptual model. This is because the conceptual model is independent of the grid and, in fact, there may be no grid at all when the conceptual model is defined. When GMS performs the ***Map->MODFLOW*** command, the return cell is always set to be the highest active cell above the drain cell. This can later be changed in the Drain package dialog.

The main DRT parameters and how they can be specified are given in the following table.

DRT Input Parameters

Parameter	Points	Nodes	Arcs	Polygons
Conductance	✓		✓	✓
Bottom elevation	✓	✓		✓
Rfprop (return-flow proportion)	✓		✓	✓

When specifying an arc as a DRT arc, the conductance and return flow factor are specified on the arc. Bottom elevation is specified at the nodes on the ends of the arc and is linearly interpolated along the length of the arc.

Care should be taken in entering conductance in the conceptual model so that the units are correct.

Drain Return package dialog

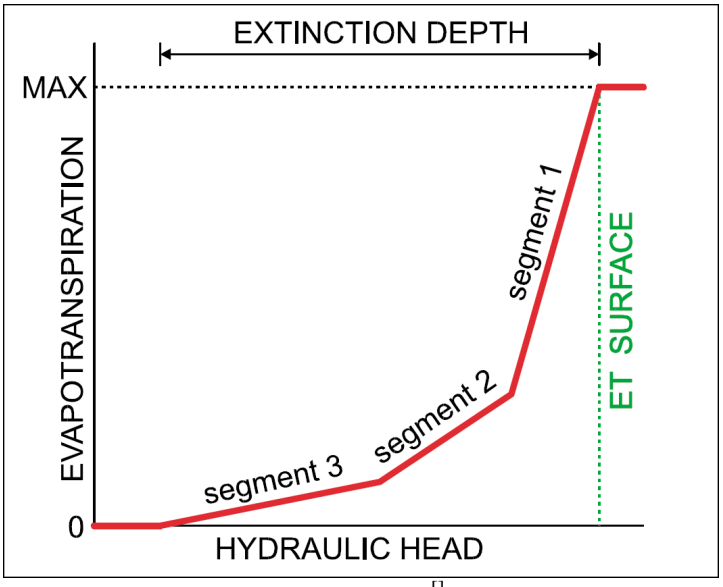
The *Drain Return package* dialog allows the user to edit the location and the input values associated with each drain boundary condition. Drain boundary conditions cannot be created or deleted from this dialog. They can be created and deleted via the ***Map -> MODFLOW*** command, or by using the *MODFLOW Source/Sink* Dialog.

The **Use Return Flow** toggle controls the existence of the "RETURNFLOW" optional keyword in the package input file.

Notes

ETS Package

The ETS package is an enhancement of the EVT package and "allows simulation of evapotranspiration with a user-defined relation between evapotranspiration rate and hydraulic head."[] It is included in MODFLOW 2000 and GMS includes an interface to it starting at version 7.0.



From OFR00-466[]

Evapotranspiration Segments

From the package documentation:

> In the ETS1 Package, the functional relation of evapotranspiration rate to head is conceptualized as a segmented line in the variable interval. The segments that determine the shape of the function in the variable interval are defined by intermediate points where adjacent segments join. The ends of the segments at the top and bottom of the variable interval are defined by the ET surface, the maximum evapotranspiration rate, and the extinction depth. The number of intermediate points that must be defined is one less than the number of segments in the variable interval. For each intermediate point, two values, PXDP and PETM, are entered to define the point. PXDP is a proportion (between zero and one) of the extinction depth, and PETM is a proportion of the maximum evapotranspiration rate. PXDP is 0.0 at the ET surface and is 1.0 at the bottom of the variable interval. PETM is 1.0 at the ET surface and is 0.0 at the bottom of the variable interval. Segments are numbered such that segment one is the segment with its upper endpoint at the ET surface, and segment numbers increase downward. The relation of evapotranspiration rate to head is defined over the model grid by a series of two-dimensional arrays; therefore, PXDP and PETM also are specified as arrays.[]

The input order of the arrays defining the segmented line is important and is defined in the package documentation:

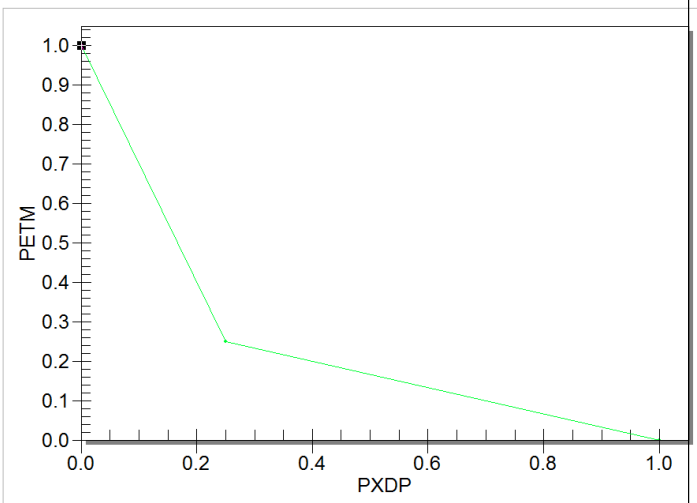
> PXDP-is a proportion of the extinction depth (dimensionless), measured downward from the ET surface, which, with PETM, defines the shape of the relation between the evapotranspiration rate and head. The value of PXDP must be between 0.0 and 1.0, inclusive. Repetitions of PXDP and PETM are read in sequence 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.
>
> 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. The value of PETM should be between 0.0 and 1.0, inclusive. Repetitions of PXDP and PETM are read 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.[]

Segmented line functions in GMS

In GMS, the ETS segmented line function can be defined in a conceptual model. When this is done, the standard XY Series Editor is used. The XY Series Editor is a simple tool for creating 2D curves. When used to define the ETS segmented function, the X values correspond to PXDP, and the Y values correspond to PETM. The order of the values is important and is defined by the package documentation as mentioned above. PXDP should be entered in order of increasing value, and PETM should be entered in order of decreasing value. Here are a couple of examples:

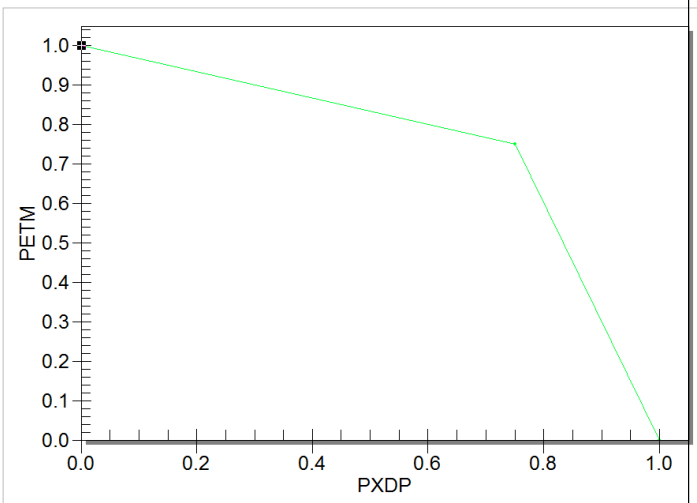
Values	Plot

PXDP	PETM
0.0	1.0
0.25	0.25
1.0	0.0



XY Series Curve 1 for ETS

PXDP	PETM
0.0	1.0
0.25	0.25
1.0	0.0



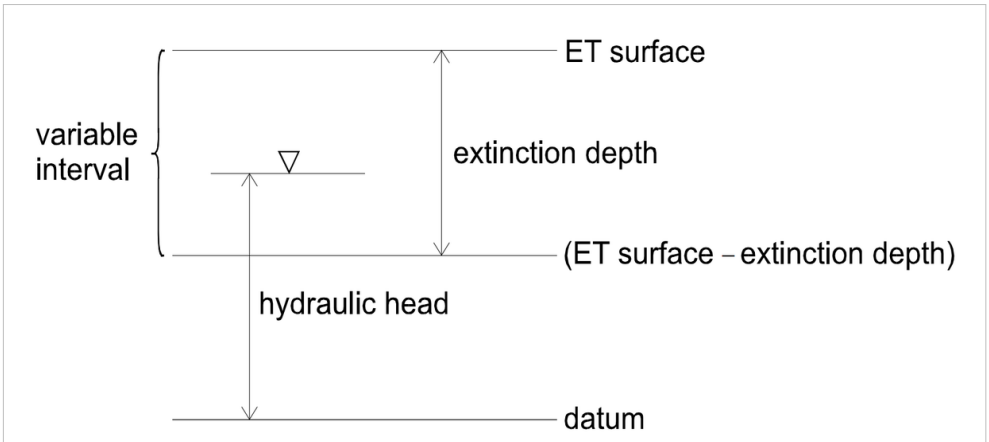
XY Series Curve 2 for ETS

In a GMS conceptual model, it is not possible to define segmented lines which vary with time. However, this can be done in the *ETS Package* dialog.

Notes

EVT Package

The Evapotranspiration package is used to simulate the effect of plant transpiration and direct evaporation by removing water from cells during a simulation. Evapotranspiration is typically defined by specifying values for each stress period for each vertical column in the grid. The values consist of an elevation, an ET extinction depth, and a maximum ET rate. The elevation is an absolute elevation and the ET extinction depth (measured positive downward) is relative to the specified elevation. If the water table rises above the specified elevation, the evapotranspiration occurs at the maximum ET rate. If the water table falls below the ET extinction depth, evapotranspiration ceases. If the water table elevation lies between these two extremes, the evapotranspiration rate varies linearly with depth. The ETS package, a later extension of the EVT package, allows the rate to vary non-linearly.



From OFR00-466[]

To learn more about Evapotranspiration in MODFLOW go here: http:/ / water. usgs. gov/ nrp/ gwsoftware/ modflow2000/ofr00-466.pdf

EVT Package Dialog

The dialog for editing the evapotranspiration package input data is identical to the Recharge Package dialog except that rather than editing the flux and layer indicator arrays, the evapotranspiration arrays are edited: elevation, ET extinction depth, maximum ET rate, and layer indicator.

Evapotranspiration Option

Two ET options are supported by MODFLOW: ET only at the top layer, and ET at specified vertical cells.

Multiplier

The multiplier is a constant which can be written to the package file with each stress period array. Each value in the array is scaled by the multiplier as the array is imported to MODFLOW. The format button brings up a dialog listing the standard MODFLOW formats. This format is used for displaying the values in the spreadsheet and it controls how the values are written to the package file.

Stress Periods

The values displayed in the spreadsheet are for an individual stress period. The values associated with other stress periods can be edited by entering the ID of the desired stress period in the Stress period edit box in the center of the dialog. If the Use previous option is selected for a given stress period, the values from the previous stress period are used and the spreadsheet is dimmed.

2D Data Set -> Array

The **2D Data Set -> Array** button brings up the Data Browser listing all of the current data sets associated with the current 2D grid. In order for this button to be active, the 2D grid must have the same number of rows and columns as the 3D grid. The selected data set is copied to the recharge array. Data sets are typically generated with the 2D Scatter Point module. The 2D Scatter Point module can be used to interpolate from a scattered set of rainfall measurements to the cell locations. If the data set is transient, the values in the data set are linearly interpolated, if necessary, to each stress period as the data set is copied to the array.

Array -> 2D Data Set

The **Array -> 2D Data Set** button copies the array to the 2D data set list associated with the existing 2D grid.

Constant -> Array

The **Constant -> Array** button brings up a dialog which prompts for a single value. This constant is then assigned to each item in the array for the given stress period.

Spreadsheet

The spreadsheet allows you to edit a 2D array of values, the type depending on the selection in the view/edit combo box. The array types include elevation, et extinction depth, and max ET rate.

Notes

GHB Package

The General Head package is similar to the Drain and River packages in that flow in or out of a cell is proportional to a difference in head. General head cells are often used to simulate lakes. General head conditions are specified by assigning a head and a conductance to a selected set of cells. If the water table elevation rises above the specified head, water flows out of the aquifer. If the water table elevation falls below the specified head, water flows into the aquifer. In both cases, the flow rate is proportional to the head difference and the constant of proportionality is the conductance.

A set of selected cells can be specified as general head cells using the ***Point Sources/Sinks*** command in *MODFLOW* menu or general heads can be assigned using the conceptual model in the Map module. When the general head attribute is assigned to a polygons, the head and conductance are applied uniformly over the entire polygon. When assigned to an arc, the conductance is applied uniformly over the arc, but separate head values are applied to each of the nodes on the ends of the arc and the head is assumed to vary linearly between the nodes. When the attribute is assigned to a point, the head and conductance values are assigned directly to the cell containing the point. Once a set of cells have been specified, the *General Head Package* dialog can be used to view and edit the values assigned to the cells.

Stress Period

The stress period field shows the current stress period and allows you to cycle through the stress periods and view the different general head properties for those stress periods in the spreadsheet below.

Use Previous

Use this option on a stress period to use the general head values from the previous stress period for the current stress period. This option is unavailable for steady state models and the first stress period of transient models.

Spreadsheet

For cells where river type boundary conditions have been assigned, the stage, conductance, bottom elevation , and conductance factor assigned to each cell are displayed in the spreadsheet portion at the lower part of the dialog. The spreadsheet can be used to edit the row, column, layer, head, and conductance values. For a transient simulation, the values displayed in the spreadsheet are for an individual stress period. The values associated with other stress periods can be edited by entering the number of the desired stress period in the stress period edit box in the center of the dialog. If the Use previous option is selected for a given stress period, the values from the previous stress period are used and the spreadsheet is dimmed. The conductance factor is used with HFB parameters. When doing parameter estimation the value of head conductance assigned to a particular head boundary condition will be the value of the head parameter multiplied by the conductance factor. For more information on HFB parameters and conductance factors see the MODFLOW 2000 manual.

Display Cell IDs/IJK

The radio group at the bottom of the dialog allows the user to adjuster whether the cell ID or the cell i, j, k values are displayed for the cells containing the boundary condition/source/sink.

Delete All

The **Delete All** button deletes all of the data currently defined in the River package and restores the River package parameters to the default values.

Global Options/Basic Package

Once the MODFLOW simulation has been initialized, the next step is to enter the data required by the Global Options/Basic package. This includes data defining fundamental program options such as the computational time intervals (stress periods), an array defining which cells are inactive and which cells have constant heads, an array of starting head values for a transient simulation, and a set of flags defining which of the other packages are to be used. The input data for this package should be entered before editing any of the other packages. The MODFLOW *Global Options\Basic Package* dialog is accessed through the ***Global Options*** command in the *MODFLOW* menu. The options in the dialog are as follows:

Headings

The two headings are optional text strings which are written to the MODFLOW text output file.

Version

The MODFLOW version can be specified with the choices being (as of July 2013):

- MODFLOW-2000
- MODFLOW-2005
- MODFLOW-NWT

The following choices will soon be added to the list:

- MODFLOW-LGR
- MODFLOW-USG

Additionally, the type of binary executable can be specified using one or more of the following choices:

- Double precision
- Parallel
- 64 bit

Run Options

The run options are not part of the actual MODFLOW input files, but present different ways that MODFLOW 2000 can be run from GMS.

Forward Run

A forward run is a normal MODFLOW simulation. If parameters have been defined for either a stochastic or parameter estimation run, the mean or starting values of the parameters are used for the forward run.

Sensitivity Analysis

The sensitivity analysis option is used to perform a sensitivity analysis on a set of selected parameters. The results can be presented with a set of plots or by contouring data sets representing grid sensitivities. This option is only available with the LPF and HUF flow packages. This option is not available in GMS 6.5 and later (see MODFLOW with HDF5).

After running PEST, sensitivities are displayed in the .sen file. Click here for more information.

Parameter Estimation

In the parameter estimation mode, a set of parameters is found that minimizes the residual between observed and simulated heads and flows. These options are described in more detail on the Automated Parameter Estimation page. This option is only available with the LPF and HUF flow packages.

Stochastic Simulation

The stochastic simulation option is used to perform a stochastic simulation using the Monte Carlo or Latin Hypercube methods for randomizing a selected set of parameters. Stochastic simulations can also be performed using a material set approach (indicator simulations). A risk analysis wizard can be used to analyze the results for a probabilistic threshold analysis or a probabilistic capture zone delineation. These options are described in more detail on the stochastic simulation page.

Stochastic Inverse Model

If the material set option is used for stochastic simulations, the "stochastic inverse" option can be used to perform automated parameter estimation on each of the N candidate model instances in the stochastic. The weighted RMS errors for each of the resulting optimized solutions can be used to weight the computations performed by the risk analysis wizard. This option is only available with the LPF and HUF flow packages.

Model Type

The simulation can be designated as either steady state or transient. If a steady state simulation is specified, certain portions of the MODFLOW interface such as the *Stress Period* dialog are inactivated since they are not relevant.

No Flow Head

This is the value of head to be assigned to all inactive (no flow) cells (IBOUND=0) throughout the simulation.

Stress Periods

The Stress Periods button is used to bring up the *Stress Period* dialog. The stress periods should be defined before any of the sources/sinks are entered. If the steady state option is selected, the **Stress Periods** button is dimmed.

Packages

The Packages button brings up the *Packages* dialog.

Units

The Units button the *Basic Package* dialog brings up the *Units* dialog.

IBOUND

Values

The IBOUND button of the *Global Options\Basic Package* dialog brings up the array editor. The IBOUND array contains a value for each cell in the grid defining the type of the cell as constant head, inactive, or variable head.

Constant Head

A negative value indicates that the cell has a constant head. The value of the constant head is defined in the starting heads array.

Inactive

An IBOUND value of zero indicates that the cell is inactive (no-flow).

Variable Head

A positive IBOUND value indicates that the cell has a variable head (i.e., the head value will be computed as part of the simulation).

Editing the IBOUND Array

There are several ways to change the active/inactive status (positive vs. zero) of a cell before or after initializing the IBOUND array. One method is to directly edit the IBOUND array using the *IBOUND* dialog. Another method is to select the ***Cell Attributes*** command in the *MODFLOW* menu. In most cases, the most efficient method is to use the ***Activate Cells in Coverage*** command in the Map module. This method uses a polygon to define the active and inactive regions.

The constant head cells are typically assigned or edited in one of three ways. One method is to directly edit the IBOUND array. Another method is to select a set of cells and use the *Cell Properties* dialog in the *MODFLOW* menu. The simplest method is to define the constant head zones using feature objects as part of a conceptual model in the Map module.

Starting Heads

The starting head values are used as initial conditions for head for both steady state and transient simulations. The **Starting Heads** button on the left side of the *Basic Package* dialog is used to enter the values of the starting heads array. Selecting the **Starting Heads** button brings up the MODFLOW Array Editor.

Top Elevation

The Top Elevation button brings up an array editor that allows you to edit the top elevation of each layer. GMS requires that the top and bottom elevations for adjacent layers be the same. This means that when you edit the bottom of one layer, move down to the next layer, and edit the top of that layer, the bottom of the previous layer will also be changed. Note that the top and bottom layer elevations must be entered regardless of the which layer data package (BCF, LPF, HUF) is chosen even though these values may not be used because of certain package options.

Bottom Elevation

The Bottom Elevation button brings up an array editor that allows you to edit the bottom elevation of each layer. Note that the top and bottom layer elevations must be entered regardless of the which layer data package (BCF, LPF, HUF) is chosen even though these values may not be used because of certain package options.

Confining Beds

The Layer Confining Beds dialog, accessed from the *Global Options/Basic Package* dialog, allows you to select which layers will have a confining bed below them. The last layer in the grid may not have a confining bed.

Confining beds are most common in older models where the user was trying to conserve memory in solving the groundwater model. In general, it is recommended that you explicitly model all of the layers in the system instead of using confining beds. This feature is supported in GMS to make it possible for users to read in older models.

In the spreadsheet, the user may turn on the confining bed option for any of the layers except the last layer in the grid.

The Confining Bed Elevations button brings up the array editor that allows the user to edit the elevation of each layer.

GMG Package

The GMG package is one of four solver packages for MODFLOW supported by GMS. The GMG solver is an iterative solver based on a multi-grid approach.

For more info on the GMG solver look at the following document: MODFLOW-2000, THE U.S. GEOLOGICAL SURVEY MODULAR GROUND-WATER MODEL -- GMG LINEAR EQUATION SOLVER PACKAGE DOCUMENTATION By: J. D. Wilson, NRC Post-Doc, and R. L. Naff, U.S. Geological Survey [1]

References

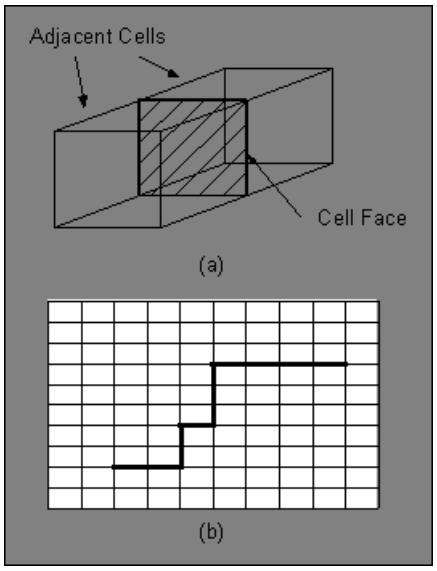
[1] http://pubs.usgs.gov/of/2004/1261/

HFB Package

The Horizontal Flow Barrier (HFB) package is used to simulate the effect of sheet pile walls, slurry trenches, or other objects which act as a barrier (or partial barrier) to horizontal flow. Barriers are simulated in the HFB package by identifying cell boundaries which approximately coincide with the location of the barrier and assigning a hydraulic characteristic to each cell boundary. Each cell boundary represents a vertical face between two adjacent cells as shown in the following figure.

Hydraulic Characteristic

The original version of the HFB Package required the input of the hydraulic characteristic either as barrier transmissivity divided by the width of the horizontal-flow barrier (for layer types 0 and 2 in BCF) or as barrier hydraulic conductivity divided by the width of the horizontal-flow barrier (for layer types 1 and 3 in BCF). In the current HFB Package, the hydraulic characteristic is always the barrier hydraulic conductivity divided by the width of the barrier, regardless of the layer type or flow package (BCF or LPF) used; thus, layer thickness is always used in calculating the contribution to the conductance terms. The HFB Package uses cell elevations specified in the discretization file to calculate cell thickness. Cell thickness is head dependent for layer types 1 and 3 in the BCF Package and for convertible layers in the Layer-Property Flow Package. (taken from MODFLOW 2000 documentation)



Cell Boundary Used to Represent Horizontal Flow Barrier. (a) Oblique View, (b) Plan View.

Defining Barriers

Barriers are defined in one of two ways: (1) they can be defined using a set of arcs in the Map module or (2) they can be defined one cell boundary at a time using the ***Toggle Barrier*** command in the 3D Grid module.

Using the Map Module

In most cases, the simplest method is to create one or more Horizontal Flow Barrier arcs in the Map module corresponding to the barriers and let GMS automatically find the closest sequence of cell boundaries and mark them as barriers.

Using the Toggle Barrier Command

Horizontal flow barriers can also be defined one at a time by selecting two adjacent cells and selecting the ***MODFLOW\Toggle Barrier*** menu command. This brings up a dialog that can be used to mark the boundary between the two selected cells as a barrier and to enter a hydraulic characteristic for the barrier. This same command can be used to delete a barrier between two cells.

HFB Package Dialog

Regardless of which method is used to define the barriers, an existing set of barriers can be viewed and edited using the ***HFB Package*** command in the *MODFLOW* menu. This command brings up the HFB Package dialog. This dialog can be used to edit the location and hydraulic characteristic of each of the currently defined barriers.

Spreadsheet

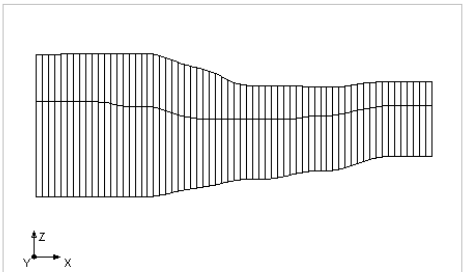
For cells where horizontal flow barriers have been assigned, the hydraulic characteristic assigned to each cell is displayed in the spreadsheet portion at the lower part of the dialog.

Reset

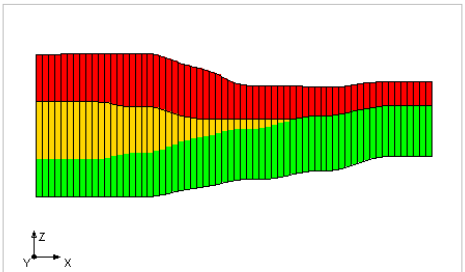
The **Reset** button can be used to delete all barriers.

HUF Package

This package is an alternative to the BCF and LPF packages. The HUF package allows the user to define the vertical elevations of the hydrogeology independent of the 3D grid as shown in the figures below. Notice in the figures below that the second grid layer has more than one hydrogeologic unit associated with it.



Side view of MODFLOW grid



HUF units displayed in MODFLOW grid

With the HUF package, the user then defines the top and thickness of each of the hydrogeologic units. A material is associated with each unit and the hydraulic properties (HK, VK...) are assigned to the material. The top and thickness arrays can be automatically generated from solids using the ***Solids -> HUF*** command from the *Solids* menu or from boreholes with the ***Horizons -> HUF*** command in the *Boreholes* menu.

Another feature in GMS that incorporates the HUF package is the ability to use TPROGS to Generate HUF Data.

Once the HUF package has been chosen using the packages dialog, the HUF package dialog can be accessed through the ***HUF package*** command in the *MODFLOW* menu. The following options are available in the HUF Package dialog.

Layer

This field displays the current layer. Selecting any of the input array buttons will display the corresponding layer initially. For multiple layer models, this field can be incremented or decremented to show other layers.

Layer type

This radio group selects the layer type for the current layer. By default, all layers are convertible.

Hydrogeologic Unit Properties

The window lists the names of the currently defined units. The Top and Thickness button bring up the MODFLOW Array Editor. For each hydrogeologic unit the user can specify if vertical hydraulic conductivity (VK) or vertical anisotropy (VANI) will be used. The material selection box show the material the is assigned to the unit. The material properties (HK, VK...) are edited by selecting the **Edit Materials** button.

Vertical hydraulic conductivity

The HUF package has the option to enter vertical hydraulic conductivity values as either actual hydraulic conductivity values or as anisotropy factors dependant on horizontal hydraulic conductivity. These options are only available for multi-layer models.

Head Assigned to Dry Cells

This is the value that MODFLOW will give to cells with a head level below the bottom elevation of the cell (dry cell). When reading in a solution, GMS will mark cells with this value with a dry cell symbol.

Cell Rewetting Parameters

If wetting of cells is allowed, a wetting factor, wetting iteration interval, and wetting equation must be specified.

LAK Package

The Lake Package is a more sophisticated alternative to the typical approach of using the General Head Package to simulate the effect of lakes and reservoirs on an aquifer. Comparing the Lake package to the GHB Package is similar to comparing the River Package to the Stream Package. With the GHB Package, the user defines the stage. With the Lake package, the stage is computed automatically based on the water budget. The water budget is a function of inflow, outflow, recharge, evaporation, etc. The storage capacity of the lake is determined automatically based on the lake geometry.Some of the cells defining the lake are allowed to go dry if the lake stage drops sufficiently.

The lake is also assumed to have lakebed sediments which affect the flow between the aquifer and the lake. The effect of the lakebed sediments is represented with a leakance term which includes the thickness and the hydraulic conductivity.

The Lake Package includes an option that allows one to simulate "sublakes". This option makes it possible for the lake to partition into smaller, separated lakes as the lake stage drops.

The Theta term offers the user a choice between an explicit solution at 0.0, a semi-implicit solution between 0.0 and 1.0, or an implicit solution at 1.0

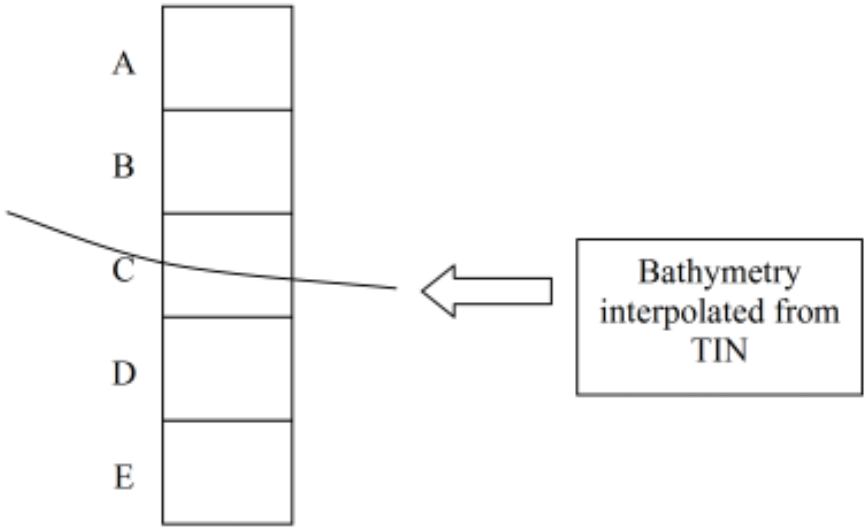
Terms

- Leakance - Represents the lakebed leakance. This is a function of hydraulic conductivity and lakebed thickness
- Bathymetry - A reference to a TIN from which the bathymetric elevations are derived.
- Sill Elev - The sill elevation at which the sublake begins to drain into the parent lake.
- Withdrawal - The volumetric rate, or flux, of water removal from a lake by means other than rainfall, evaporation, surface outflow, or ground-water seepage.

Adjust Cell Elev.

Lake polygons in a conceptual model include an option called "Adjust Cell Elev." This option often results in thin cells and instability and should generally be avoided. Here's how it works. GMS interpolates a bathymetric elevation from the appropriate TIN and finds the cell where the top of the cell is above the bathymetric elevation and the bottom of the cell is below. After finding the intersecting cell, all cells above the point in question are marked as inactive (IBOUND = 0) and assigned with the appropriate lake ID. For the cell that intersects the bottom of the lake, the way the cell is handled depends on what layer it is in. If the cell is in the top layer, it is made inactive, marked as part of the lake, and the bottom elevation of the cell is adjusted to match the lake bottom. If the cell is in one of the lower layers, GMS first determines if the lake bottom is closer to the top of the cell or the bottom of the cell. If the

lake bottom is closer to the top of the cell, the top elevation for the cell is adjusted to match the bottom of the lake and the cell is left as active and NOT marked as being in the interior of the lake. If the lake bottom is closer to the bottom of the cell, the bottom elevation of the cell is adjusted to match the lake bottom and the cell is marked as both inactive and inside of the lake.



LMG Package

The LMG1 package is only supported in GMS versions prior to 8.0. The LMG1 Package information can be found here.

LMG3 package offers some improvements over the LMG1 package for certain types of problems. The LMG3 package is backward compatible with LMG1 input files. For non-linear problems and simulations which use several time steps, subsequent matrices to be solved for often change only slightly in their algebraic properties. In this case the LMG3 offers a possibility to accelerate the overall simulation time enormously.

MXITER. Maximum outer iterations

This value is the maximum iterations, or calls to the solver. For linear problems, this value can be 2. For non linear problems, this values should be larger, but generally less than 50.

MXCYC. Maximum inner iterations

This value is the maximum number of iterations per call to the solver. The default value is 50, and this is sufficient for most problems.

RCLOSE. Inner iteration closure criterion

Same as RCLOSE for the GMG solver package. The PCG algorithm computes the l2norm of the residual and compares it against RCLOSE. In LMG1 this was called Budget Closure Criterion. When the scaled norm of the matrix equations is less than this value then the solver iteration stops.

HCLOSE. Outer iteration closure criterion

Head change convergence criterion for nonlinear problems. After each linear solve (inner iteration), the maximum norm of the head change is compared against HCLOSE.

CONTROL. LMG version to use

This variable allows the user to select either LMG1 or LMG2 version of the LMG solver.

Damping method

Three different damping methods are available: constant, Adaptive damping using the Cooley method, or Adaptive RRR damping using the relative reduced residual. Refer to the official package documentation for more explanation on the different damping methods.

DAMP. Accleration Parameter

This value is used if the acceleration method is set to constant. Usually, this value is 1.0, but for some problems lower values may help achieve convergence.

DUP. Max Acceleration

This is the max damping value when using the adaptive damping with relative reduced residual.

DLOW. Min Acceleration

This is the min damping value when using the adaptive damping with relative reduced residual.

Conjugate Gradient

Controls whether the conjugate gradient method is used to accelerate the solver. By default this option is on.

Stor1, Stor2, Stor3

These values are ignored in LMG2. In LMG1, these variables are used to control the amount of memory storage used by the solver. The defaults rarely need to be changed.

IOUTAMG. Output control

This controls the information printed to the samg output file while the solver is running.

Reset

This button will change all options to the default state.

LMG1 Package

The LMG package is one of four solver packages for MODFLOW supported by GMS.

Maximum outer iterations

This value is the maximum iterations, or calls to the solver. For linear problems, this value can be 2. For non linear problems, this values should be larger, but generally less than 50.

Maximum inner iterations

This value is the maximum number of iterations per call to the solver. The default value is 50, and this is sufficient for most problems.

Acceleration type

Three different acceleration methods are available: constant, adaptive damping using the Cooley method, or adaptive damping using the relative reduced residual. Refer to the official package documentation for more explanation on the different damping methods.

Accleration Parameter

This value is used if the acceleration method is set to constant. Usually, this value is 1.0, but for some problems lower values may help achieve convergence.

Max Acceleration

This is the max damping value when using the adaptive damping with relative reduced residual.

Min Acceleration

This is the min damping value when using the adaptive damping with relative reduced residual.

Budget Closure Criterion

When the scaled norm of the matrix equations is less than this value then the solver iteration stops.

Conjugate Gradient

Controls whether the conjugate gradient method is used to accelerate the solver. By default this option is on.

Stor1, Stor2, Stor3

These variables are used to control the amount of memory storage used by the solver. The defaults rarely need to be changed.

Reset

This button will change all options to the default state.

LPF Package

This package is an alternative to the BCF and HUF packages and is similar to the "true layer" option used with the BCF package in version 3.1. With MODFLOW 2000, the layer elevations (top and bottom) are defined as input to the Global Process (using the Global Options Dialog), regardless of which flow package is being used. With the LPF package, the user then defines the horizontal and vertical hydraulic conductivity for each layer. MODFLOW then computes the cell by cell conductances using the K values and the layer geometry.

Other noteworthy features include the ability to enter horizontal anisotropy values on a cell by cell basis. There is also an option to specify vertical anisotropy factors rather than vertical hydraulic conductivity values. This option is particularly useful when performing automated parameter estimation since it ties the K_v to K_h and eliminates the need to define K_v as an independent parameter.

Another feature of the LPF package relative to the BCF package is that there are now only two layer types: confined and convertible. A convertible layer is similar to the LAYCODE = 2 and LAYCODE = 3 types in the BCF package. The layer can be either confined or unconfined depending on the elevation of the computed water table.

Once the LPF package has been chosen using the packages dialog, the LPF package dialog can be accessed through the LPF package command in the *MODFLOW* menu.

Use data arrays

This option allows you to enter conductivities on a layer-by-layer basis. When this option is chosen, the Horizontal Hyd. Conductivity…, Vertical Hyd. Conductivity, Specific Storage, etc. buttons will be available.

Use material ids

This options uses material sets in the place of property arrays. Property values are entered on a material-by-material basis. When MODFLOW files are saved, GMS internally replaces the correct values from the materials to the property arrays. When this option is chose, the property array buttons are replaced with the **Material Properties** and **Material IDs** buttons.

Layer

This field displays the current layer. Selecting any of the input array buttons will display the corresponding layer initially. For multiple layer models, this field can be incremented or decremented to show other layers.

Layer type

This radio group selects the layer type for the current layer. By default, all layers are convertible. Here you can change the layer type to confined.

Vertical hydraulic conductivity

The LPF package has the option to enter vertical hydraulic conductivity values as either actual hydraulic conductivity values or as anisotropy factors dependant on horizontal hydraulic conductivity. Vertical anisotropy (VKA) "is the ratio of horizontal to vertical hydraulic conductivity. In this case, HK is divided by VKA to obtain vertical hydraulic conductivity, and values of VKA typically are greater than or equal to 1.0."[1] These options are only available for multi-layer models.

Interblock transmissivity

The method used for computing interblock transmissivity is specified using the pull-down list in the middle right portion of the *LPF Package* dialog.

Layer Data Arrays

The eight buttons in the lower right portion of the dialog represent layer data arrays such as elevations and hydraulic conductivity. Each of the eight buttons brings up the MODFLOW Array Editor. Not all of the data arrays need to be specified for each layer. Some arrays such as Specific Storage and Specific Yield are only required for transient models.

Head Assigned to Dry Cells

This is the value that MODFLOW will give to cells with a head level below the bottom elevation of the cell (dry cell). When reading in a solution, GMS will mark cells with this value with a dry cell symbol.

Remove vertical leakance correction

This is the value that MODFLOW will give to cells with a head level below the bottom elevation of the cell (dry cell). When reading in a solution, GMS will mark cells with this value with a dry cell symbol. The Layer Property Flow Package of MODFLOW-2000 was modified by A.W. Harbaugh (U.S. Geological Survey, written commun., 2002) to remove the vertical leakage correction for conditions in which a partially saturated cell is immediately below a fully or partially saturated cell (Harbaugh and others, 2000, p. 31-33). The vertical leakage correction simulates perched conditions within an aquifer system. However, perched conditions are not known to be widespread on a basin scale. The vertical leakage correction adds an additional nonlinear term to the model (A.W. Harbaugh, U.S. Geological Survey, written commun., 2002), which resulted in several of the numerical solvers (SIP (strongly implicit procedures), SOR (slice-successive overrelaxation), and PCG (Hill, 1990; Harbaugh and others, 2000) not coming to a solution and the LMG (link-algebraic multigrid; Mehl and Hill,2001) solver providing unacceptable volumetric budget errors (wrir02-4200.pdf) . Thus in the LPF package the user has the option to turn off the vertical leakance correction to account for these factors. As the user turns on the "Remove Vertical Leakance Correction" toggle, GMS then uses the NOCVCORRCTION [2] option that is found in MODFLOW2005 to remove vertical leakance corrections.

Cell Rewetting Parameters

If wetting of cells is allowed, a wetting factor, wetting iteration interval, and wetting equation must be specified.

Notes

[2] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/index.html?lpf.htm

MNW1 Package

The Multi-Node Well (MNW1) package was developed to more accurately model wells that are completed in multiple aquifers or in a single heterogeneous aquifer, partially penetrating wells, and horizontal wells that can be affected by the effects of dynamic changes in the distribution of pumping or intraborehole flow that can significantly alter groundwater flow. A more recent revision of the MNW package is available in the MNW2 package. A MODFLOW model can not use both the MNW1 and MNW2 packages, it must use one or the other.

MNW1 boundary conditions can be added to selected cells using the ***Point Sources/Sinks*** command in the *MODFLOW* menu. MNW1 points can also be defined using the conceptual model approach in the map module.

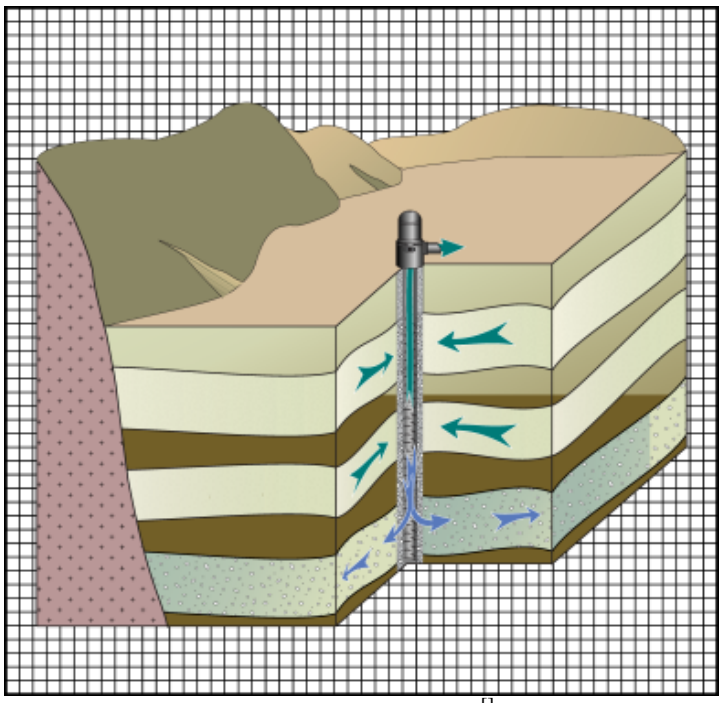


Illustration of MNW package[]

Conceptual model

MNW1 Wells can be modeled using points in a conceptual model. The user can specify the various MNW1 properties associated with points in a coverage. In addition, a multi-node MNW1 boundary condition (bc) can be created using the conceptual model approach. The easiest way to create a multi-node MNW1 bc is to define a well screen associated with the MNW1 point that crosses multiple layers of the MODFLOW grid. Another method for creating a multi-node MNW1 bc is to specify a common "Well ID" to group different points together. Thus, multiple points in the same or different coverages can be used to create multi-node MNW1 bcs.

Multi-Node Well package dialog

The Multi-Node Well (MNW1) package dialog allows the user to edit the location and the input values associated with each mnw boundary condition. MNW1 boundary conditions cannot be created or deleted from this dialog. They can be created and deleted via the ***Map -> MODFLOW*** command, or by using the *MODFLOW Source/Sink* Dialog.

The upper section of the dialog controls global options for the package. The spreadsheet in the lower section of the dialog controls the bcs that vary with each stress period. The user is referred to the MNW1 documentation for a full explanation of each of the inputs to the MNW1 boundary conditions. In GMS we have added the Name, Active, and Well ID fields. Name is a label used to identify a boundary condition. Active is a flag used to determine if the boundary condition is used during a particular stress period. The Well ID field is used to identify multi-node wells.

Notes

MNW2 Package

The Multi-Node Well (MNW2) package is an updated revision of the MNW package meant to replace the MNW1 Package. It includes modifications to better model partially penetrating wells, non-vertical wells, and includes the ability to specify a pump performance curve. The MNW package was developed to more accurately model wells spanning multiple aquifers or in a single heterogeneous aquifer, partially penetrating wells, and horizontal wells that can be affected by the effects of dynamic changes in the distribution of pumping or intraborehole flow that can significantly alter groundwater flow. A MODFLOW model can not use both the MNW1 and MNW2 packages, it must use one or the other. A detailed description of the MNW2 input is available at the USGS website [28].

MNW2 boundary conditions can be directly added via the Multi-Node well (MNW2) package dialog. Boundary conditions can also be added to selected cells using the ***Point Sources/Sinks*** command in the *MODFLOW* menu. For a conceptual model MNW2 points can be defined in the map module.

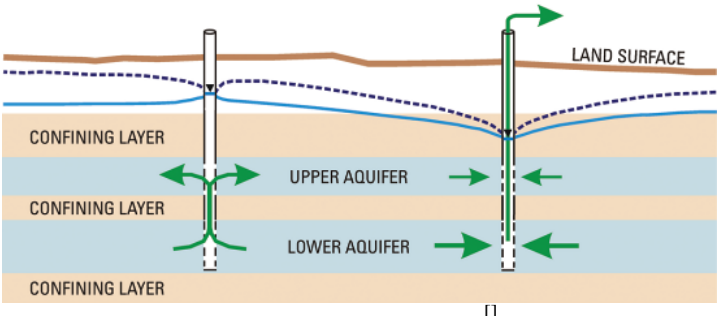


Illustration of MNW2 package[]

Conceptual Model

An MNW2 well can be added to a conceptual model by creating an MNW2 point. The geometry of the well screen can be set using the **Use screen** attribute for a single screen, or for multiple screens the geometry can be set using the **Boreline** attribute button. If niether one is set, the generated well nodes include the grid layers specified for the coverage by its default layer range.

Multi-Node Well (MNW2) Package Dialog

MNW2 Wells can be edited in the *Multi-Node Well (MNW2) Package* Dialog. The main dialog allows editing stress period data for wells. The stress period field shows the current stress period and allows you to cycle through stress periods and view the well properties for each stress period in the spreadsheet below. MNW2 AUX fields can be added and removed by clicking on the **Edit AUX...** button. The values are displayed in the spreadsheet. Controls to edit the print detail (MNWPRNT) and the MNWI package values are available below the spreadsheet. Wells can be added, edited and removed by clicking on the **Wells...** button to bring up the MNW2 Wells Dialog.

MNW2 Wells Dialog

The *MNW2 Wells* Dialog allows wells to be added, removed, and edited. It consists of two spreadsheets. The top spreadsheet lists the table of MNW2 wells. When a well in the top spreadsheet is clicked on, the nodes for the well are listed in the bottom spreadsheet. Nodes can be added and removed by changing the NNODES column in the wells spreadsheet.

Sources/Sinks Dialog

An MNW2 well can be added or edited for a selected cell using the *Sources/Sinks* menu item under the *MODFLOW* menu. The well info can be edited from the Sources/Sinks Dialog by clicking on the button in the Edit column.

Notes

NWT Package

The Newton package (NWT) is one of the solvers available in MODFLOW-NWT. The NWT package is only used with the UPW Package. Using the NWT solver requires twice the memory of other MODFLOW solvers because using the Newton method results in an asymmetric matrix. Because of the asymmetric matrix a different matrix solver must be used. The NWT package provides an option to use one of two matrix solvers: a generalized-minimum-residual (GMRES) solver and an Orthomin/stabilized conjugate-gradient solver called *x*MD (chi-MD).

For more information on the NWT package see the USGS documentation here. [16]

PCG2 Package

The PCG2 package is one of four solver packages for MODFLOW supported by GMS.

Maximum outer iterations

This value is the maximum iterations, or calls to the solver. For linear problems, this value can be 1, unless more than 50 inner iterations are required, when maximum outer iterations could be as large as 10. For non linear problems, this values should be larger, but generally less than 100.

Maximum inner iterations

This value is the maximum number of iterations per call to the solver. The default value is 50, and this is sufficient for most problems.

Matrix Preconditioning Method

Use this radio group to choose the matrix conditioning method. The default is to use a modified incomplete cholesky method.

Relaxation Parameter

This value is used if the modified incomplete cholesky method is used. Usually, this value is 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.

Head Change Criterion For Convergence

When the maximum absolute value of head change from all cells during an iteration is less than or equal to the head change criterion, AND the residual change criterion is met, solver iteration stops.

Residual Change Criterion For Convergence

When the maximum absolute value of residuals from all cells during an iteration is less than or equal to the residual change criterion, AND the head change criterion is met, solver iteration stops.

Reset

This button will change all options to the default state.

RCH Package

The Recharge package is used to simulate recharge to an aquifer due to rainfall and infiltration. Recharge is typically defined by specifying a recharge value for each stress period for each vertical column in the grid (i.e., a NLAY X NCOL array of values is entered). The recharge value represents the amount of water that goes into the groundwater system and not the amount of precipitation. The units of recharge are length/time, so in a cell with a recharge value of 10(m/day), 10 meters of rainfall each day would be distributed across every m^2 of the cell. The recharge parameters are specified in the Recharge Package dialog. The options in the dialog are as follows:

Recharge Option

Three recharge options are supported by MODFLOW: recharge only at the top layer, recharge at specified vertical cells, and recharge at highest active cells.

Multiplier

The multiplier is a constant which can be written to the package file with each stress period array. Each value in the array is scaled by the multiplier as the array is imported to MODFLOW. The format button brings up a dialog listing the standard MODFLOW formats. This format is used for displaying the values in the spreadsheet and it controls how the values are written to the package file.

Stress Periods

The values displayed in the spreadsheet are for an individual stress period. The values associated with other stress periods can be edited by entering the ID of the desired stress period in the Stress period edit box in the center of the dialog. If the Use previous option is selected for a given stress period, the values from the previous stress period are used and the spreadsheet is dimmed.

Layer Indicator

If the Recharge at specified vertical cells option is chosen, the layer indicator for each vertical cell can be displayed and edited in the spreadsheet window by selecting Layer indicator in the View/Edit option.

Constant -> Array

The **Constant -> Array** button brings up a dialog which prompts for a single value. This constant is then assigned to each item in the array for the given stress period.

2D Data Set -> Array

The **2D Data Set -> Array** button brings up the Data Browser listing all of the current data sets associated with the current 2D grid. In order for this button to be active, the 2D grid must have the same number of rows and columns as the 3D grid. The selected data set is copied to the recharge array. Data sets are typically generated with the 2D Scatter Point module. The 2D Scatter Point module can be used to interpolate from a scattered set of rainfall measurements to the cell locations. If the data set is transient, the values in the data set are linearly interpolated, if necessary, to each stress period as the data set is copied to the array.

Array -> 2D Data Set

The **Array -> 2D Data Set** button copies the array to the 2D data set list associated with the existing 2D grid.

Spreadsheet

The recharge flux values for each of the vertical columns in the grid are displayed and edited in the spreadsheet at the lower part of the dialog.

Reset

The **Reset** button deletes all of the data currently defined in the package and restores the package parameters to the default values.

PEST ASP Package

Prior to version 9.0 this command and dialog were called "Convergence Options".

When performing automated parameter estimation, a set of optimal parameter values can only be found if MODFLOW produces a stable solution for all iterations. One of the things that can cause problems with the inverse model is cells going dry. The dry cell flag that is written to the head array can cause instability in the inverse model, and thus it will not converge. When such problems occur, a successful run may be achieved by turning on some convergence options that have been added to the GMS version of MODFLOW by John Doherty. These options are accessed via the ***PEST ASP Package*** command in the *MODFLOW* menu. The options are as follows:

Do Not Stop on Non-Convergence

The "Do not stop ..." option is used for transient simulations. When this option is on, if the MODFLOW model does not converge for a particular time step, it continues to the next time step rather than aborting.

Assign Bottom Elevation to Dry Cells

During a normal MODFLOW run, if a cell goes dry, the HDRY value assigned in the BCF package is assigned to the cell. The default value for HDRY is -888. At each iteration of the inverse model run (each time a MODFLOW solution is found), the inverse model interpolates the computed head values to the observation points and computes the residual error. This error is factored into the objective function. If the head at a cell near an observation point suddenly switches from a normal head value to -888, an extreme discontinuity is introduced to the objective function and the inverse model may not be able to converge. This problem can be avoided by turning on the Assign bottom elevation to dry cells option. If this option is on, the bottom elevation associated with the cell is assigned as the head value for the cell.

Prevent Cell Drying

The Prevent Cell Drying option does not allow a cell in the bottom layer to go dry. The head is not allowed to drop below the value corresponding to the specified minimum saturated thickness. Additional instruction is provided by Richard Winston and in a USGS Open-File [1]:

> Use of the wetting capability can cause serious problems with convergence. You can try to avoid this by several methods.

1. If you know a cell should never become wet, make it an inactive cell rather than a variable head cell.
2. You can adjust the value of the wetting threshold in WETDRY. (Higher is more stable but may be less accurate.)
3. You can decide which neighbors will be checked to decide if a cell should be wetted using WETDRY. Often it is better to allow only the cell beneath the dry cell to rewet it.
4. You can use IHDWET to determine which equation is used to specify the head in newly wetted cells.
5. You can vary the wetting factor WETFCT.
6. In steady-state conditions you can adjust initial conditions to values that are close to your best guess of the final conditions to improve stability.
7. You can choose a different solver. The SIP, PCG1, and PCG2 solvers will work with the wetting capability. The SOR solver doesn't work well with the wetting capability. Note that cells can not change between wet and dry during the inner iterations of the PCG1 and PCG2 solvers. The PCG1 solver is no longer included in the USGS version of MODFLOW.
8. When using the PCG2 solver, you can set RELAX in the range of 0.97 to 0.99 to avoid zero divide and non-diagonally dominant matrix errors. (However, this is an infrequent cause of instability. If such an error occurs, PCG2 prints an error message in the output file and aborts the simulation.)
9. When using the PCG2 solver, you can set DAMP to a value between 0 and 1.
10. Unrealistically high conductances on boundary cells can contribute to instability. Check the conductances in the Drain, River, Reservoir, Lake, Stream, and General-Head Boundary packages. In the Evapotranspiration check the EVT Flux Stress[i] and EVT Extinction Depth which together control the conductance of evapotranspiration cells.

> The two most important variables that affect stability are the wetting threshold and which neighboring cells are checked to determine if a cell should be wetted. Both of these are controlled through WETDRY. It is often useful to look at the output file and identify cells that convert repeatedly from wet to dry. Try raising the wetting threshold for those cells. It may also be worthwhile looking at the boundary conditions associated with dry cells.
>
> Sometimes cells will go dry in a way that will completely block flow to a sink or from a source. After that happens, the results are unlikely to be correct. It's always a good idea to look at the flow pattern around cells that have gone dry to see whether the results are reasonable.

References

[1] http://pubs.er.usgs.gov/usgspubs/ofr/ofr91536

RIV Package

A set of selected cells can be specified as river cells using the ***Point Sources/Sinks*** command in the *MODFLOW* menu or river cells can be created using the conceptual model in the Map module. River attributes are typically used with arcs but may also be associated with polygons and points. The river parameters include elevation, stage, and conductance. Elevation is constant. The river stage and conductance may either be constant or vary with time.

When the river attribute is assigned to an arc, the conductance is applied uniformly over the arc, but separate elevations and stage values are applied to each of the nodes on the ends of the arc, and the elevation and stage are assumed to vary linearly between the nodes. When a river object is defined using a polygon or a point, all of the values are assigned directly to the cell(s) overlapped by the polygon or point.

Once a set of river cells has been specified, the *MODFLOW River Package* dialog can be used to view and edit the values assigned to the cells. The options in the dialog are as follows:

Stress Period

This field shows the current stress period and allows you to cycle through the stress periods and view the different river properties for those stress periods in the spreadsheet below.

Spreadsheet

For cells where river type boundary conditions have been assigned, the stage, conductance, bottom elevation, and conductance factor assigned to each cell are displayed in the spreadsheet portion at the lower part of the dialog. The spreadsheet can be used to edit the row, column, layer, stage, conductance, and bottom elevation values. For a transient simulation, the values displayed in the spreadsheet are for an individual stress period. The values associated with other stress periods can be edited by entering the number of the desired stress period in the stress period edit box in the center of the dialog. If the Use previous option is selected for a given stress period, the values from the previous stress period are used and the spreadsheet is dimmed. The conductance factor is used with RIV parameters. When doing parameter estimation the value of river conductance assigned to a particular river boundary condition will be the value of the river parameter multiplied by the conductance factor. For more information on RIV parameters and conductance factors see the MODFLOW 2000 manual.

SIP Package

The SIP package is one of four solver packages for MODFLOW supported by GMS.

Maximum Iterations Per Time Step

This value is the maximum number of times through the iteration loop in one time step in an attempt solve the system of finite-difference equations.

Number of Iteration Parameters

Five variables are generally sufficient.

Acceleration Parameter

This value must be greater than zero and is usually 1.0.

Head Change Criterion For Convergence

When the maximum absolute value of head change from all cells during an iteration is less than or equal to the head change criterion, solver iteration stops.

Print Out Interval

The maximum absolute head change is printed for each iteration of a time step whenever the time step is an even multiple of the print out interval. The printout also occurs at the end of each stress period regardless of the print out interval.

Iteration Parameter Seed

These options control the seed for calculating iteration variables. You can either specify the seed yourself or have MODFLOW calculate it.

Reset

This button will change all options to the default state.

SSOR Package

The SSOR package is one of four solver packages for MODFLOW supported by GMS. The SOR solver only uses a head change convergence criterion and may result in significant volume budget error.

Maximum iterations per time step

This value is the maximum solver iterations per timestep. The default value is 50.

Acceleration Parameter

This value is usually between 1.0 and 2.0

Head change criterion for convergance

When the maximum absolute value of head change from all cells during an interation is less than or equal to the head change criterion, solver iteration stops.

Print out interval

The maximum absolute head change is printed for each iteration of a time step whenever the time step is an even multiple of the print out interval. The printout also occurs at the end of each stress period regardless of the print out interval.

Reset

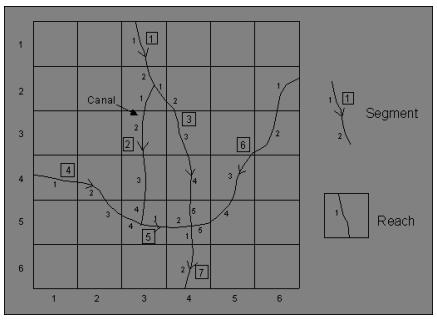
This button will change all options to the default state.

STR/SFR Packages

The STR and SFR packages are used to simulate the interaction between surficial streams and the groundwater. These packages are somewhat similar to the River package in that water can move from the stream to the aquifer or from the aquifer to the stream depending on the relative differences in the stream stage and the water table elevations. However, unlike the River package, flow is routed through the stream. For the STR package, simple channel hydraulics and Manning's equation are used to compute the stage in the stream. The SFR package has more sophisticated hydraulics and routing options.

Stream Network

When either the STR or SFR package is used, a complete, ordered stream network must be defined as shown in the following figure.



Ordered stream network used by the STR or SFR packages.

A stream network is composed of reaches and segments. A reach is the portion of a stream that lies inside a single cell. A single cell may contain multiple reaches. A segment is a group of reaches that forms one section of the stream. The reaches within a segment are always numbered from upstream to downstream. The segments should also be numbered from upstream to downstream.

The incoming flowrate may only be defined for the topmost segments (segments 1, 4, and 6 in the above figure) and is typically entered as a positive value to represent the amount of flow in the stream channel. Flow is then routed and combined to get the incoming flowrate for the other segments. An exception to this is a diversion such as the canal at segment #2 in the above figure. In this case the flowrate into the diversion should be specified. The flow to the diversion would be subtracted from the flow coming out of segment #1 and whatever is left over would be routed to segment #3.

Defining Streams

Unlike other packages in GMS, a stream network cannot be created by selecting cells in the grid and manually assigning values to the cells. Due to the complex nature of the input and the requirement that the data be ordered in a specific fashion, a stream network can only be created using a series of Stream Arcs in the Map module. The cell-by-cell values are automatically created and properly ordered when the ***Map -> MODFLOW*** command is selected.

There are some restrictions on the STR and SFR conceptual models:

- STR and SFR stream arcs cannot both exist in the same coverage because of the stream numbering issues.
- All STR (or SFR) arcs must be in one coverage. You cannot use two or more coverages to represent your stream network.
- SFR - All downstream streams must be diversions except for one. The variable OUTSEG is the segment number of the downstream segment that is not a diversion.
- SFR - If the current segment has the diversion flag set then IUPSEG is the id of the upstream segment.

Set Arc Directions From Stream Data

Right-clicking on a coverage containing STR streams shows a *Set Arc Directions From Stream Data* menu item. This operation will cause all stream arcs to point downhill based on the elevation of the top of the river sediments as defined at the nodes.

STR Package

In the input file for the STR package, each reach is assigned the following values:

- ijk indices of cell
- segment ID
- reach ID
- stage (typically starting stage)
- conductance
- conductance factor (multipled by the conductance during parameter estimation)
- Elevation of the bottom of the streambed
- Elevation of the top of the streambed

Each segment is assigned the following values:

- incoming flow (for top segments and diversions)
- width
- slope
- roughness coefficient
- IDs of tributaries (upstream segments)
- ID of upstream segment (for diversions only)

When Manning's equation is used to route the flow through the network, the stream channels are assumed to have a rectangular cross section.

When the Map -> MODFLOW command is selected, GMS automatically does the following: classifies all of the cells beneath the streams as reaches, builds segments, numbers the reaches and segments, and assigns the appropriate values to the reaches and segments. These values defined at the nodes are linearly interpolated across the arcs when the model is converted. The slope assigned to reaches is computed by dividing the difference in the streambed top elevations at the ends of the arc by the arc length multiplied by the sinuosity factor.

The STR Package Dialog

Once the ***Map -> MODFLOW*** command is selected and the stream data have been assigned to the grid cells, the data can be viewed and some of the input values can be edited using the *Stream Package* dialog. The options for the Stream Package dialog include:

Calculate Stage

The Calculate stage toggle is used to specify whether the Stream package should compute the stages (specified stages are initial values only) or whether the specified stages should be used directly.

SFR Package

Support for the SFR2 package was added at GMS version 7.0.

The SFR Package Dialog

Once the ***Map -> MODFLOW*** command is selected and the stream data have been assigned to the grid cells, the data can be viewed and some of the input values can be edited using the SFR Package dialog. Stream segments and reaches cannot be created in the *SFR Package* dialog - creation can only be done via the ***Map -> MODFLOW*** command. The *SFR Package* dialog has two spreadsheets, one showing stream segments and one showing stream reaches. For a further explanation of the columns in each spreadsheet you can refer to the Online Guide to MODFLOW [31].

ISTCB2 info

If the *Save ISTCB2 info to *.istcb2 text file* option is on, MODFLOW will save more stream related data to a text file which has the same prefix as the other MODFLOW files and a "*.istcb2" extension. This text file will be displayed in the MODFLOW Solution in the Project Explorer when the solution is imported. The data in this file includes information on "inflows and outflows from each reach; on stream depth, width, and streambed conductance; and on head difference and gradient across the streambed."

If the *Save ISTCB2 info to *.istcb2 text file* option is off, streamflow out of each reach will be saved to the CCF file if the *Save cell by cell flow terms to *.ccf file* is on in the*Output Control* dialog.

Starting at GMS 9.0, this information is saved to a second CCF file that will appear in the solution as "CCF2". This is so that the stream flow out of each reach is not included in the flows in and out of the aquifer in the flow budget. The total stream flow out of each reach is displayed at the bottom of the flow budget.

STREAMFLOW_OUT data set

The stream flow out of each reach is stored in the ccf file under the heading STREAMFLOW_OUT. GMS can convert data in the CCF file to 3D grid data sets that can be contoured by right-clicking on the CCF file in the *Project Explorer* and using the *CCF -> Data Sets* command. If in the ccf file multiple flows are listed for the same cell, GMS sums them so that there is only one value for each cell in the resulting data set. With most data this makes sense because the data represents the total flow into our out of the aquifer due to the BC (wells, river etc). The STREAMFLOW_OUT data is treated the same way, but in this case it doesn't make sense to sum the values because they don't represent flow to or from the aquifer. The problem becomes evident wherever there is more than one stream reach in a cell, which happens wherever a stream segment begins/ends in a cell. The STREAMFLOW_OUT data set value will be the sum of all the reaches in the cell, which can make it appear as if much more water is flowing down the stream than there should be in that cell. If using SFR2 you should save the istcb2 data as a text file (described above) which lists the streamflow out of each segment and reach separately. Despite this problem, the STREAMFLOW_OUT data set can still be useful for contouring and display purposes.

UZF Package

The UZF Package is used to simulate percolation of water through the unsaturated zone. This package is compatible with MODFLOW 2005 (not earlier versions of MODFLOW).

The inputs to the UZF Package are edited in the UZF Package dialog. The inputs to the UZF package are explained here [1]. All of the inputs are labeled using the MODFLOW variable names.

Gages

The spreadsheet with the IUZROW, IUZCOL, IFTUNIT, and IUZOPT columns is used to edit gages associated with the UZF package. By default GMS will assign the unit numbers to the gage files (the IFTUNIT variable). However, the user can specify these values by turning on the toggle below the spreadsheet and entering the unit numbers in the IFTUNIT column. Gages can be added or removed by selecting the insert or delete buttons below this spreadsheet.

Care should be taken to enter unique unit numbers. The user can inspect the MODFLOW name file (*.mfn) written by GMS to ensure that the specified unit numbers are unique.

Multiplier

The multiplier is a constant which can be written to the package file with each array. Each value in the array is scaled by the multiplier as the array is imported to MODFLOW.

Stress Periods

The values displayed in the spreadsheet are for an individual stress period for the first 4 arrays (FINF, PET, EXTDP, and EXTWC). The other arrays are not specified per stress period.

The values associated with different stress periods can be edited by entering the ID of the desired stress period in the Stress period edit box. If the Use previous option is selected for a given stress period, the values from the previous stress period are used and the spreadsheet is not editable.

Constant -> Array

The **Constant -> Array** button brings up a dialog which prompts for a single value. This constant is then assigned to each item in the array for the given stress period.

2D Data Set -> Array

The **2D Data Set -> Array** button brings up the Data Browser listing all of the current data sets associated with the current 2D grid. In order for this button to be active, the 2D grid must have the same number of rows and columns as the 3D grid. The selected data set is copied to the recharge array. Data sets are typically generated with the 2D Scatter Point module. The 2D Scatter Point module can be used to interpolate from a scattered set of rainfall measurements to the cell locations. If the data set is transient, the values in the data set are linearly interpolated, if necessary, to each stress period as the data set is copied to the array.

Array -> 2D Data Set

The **Array -> 2D Data Set** button copies the array to the 2D data set list associated with the existing 2D grid.

Spreadsheet

The values for the array listed in the View/Edit selection box are shown in the spreadsheet.

References

[1] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/uzf_unsaturated_zone_flow_pack.htm

WEL Package

A set of selected cells can be specified as wells using the ***Point Sources/Sinks*** command in the *MODFLOW* menu or by using the conceptual model in the Map module. Wells are specified by assigning a pumping rate to a selected cell at the location of each well. Wells can be either injection wells (positive flow rate) or extraction (negative flow rate) wells.

Once a set of cells has been specified, the *Well Package* dialog can be used to view and edit the values assigned to the cells.

Stress Period

The stress period field shows the current stress period and allows you to cycle through the stress periods and view the different well properties for those stress periods in the spreadsheet below.

Use Previous

Use this option on a stress period to use the well values from the previous stress period for the current stress period. This option is unavailable for steady state models and the first stress period of transient models.

Spreadsheet

For cells where well type boundary conditions have been assigned, the well flow rate for each cell is displayed in the spreadsheet portion at the lower part of the dialog. The spreadsheet can be used to edit the well name, row, column, layer, and flow values.

For a transient simulation, the values displayed in the spreadsheet are for an individual stress period. The values associated with other stress periods can be edited by entering the number of the desired stress period in the stress period edit box in the center of the dialog. If the Use previous option is selected for a given stress period, the values from the previous stress period are used and the spreadsheet is dimmed.

The conductance factor is used with WEL parameters. When doing parameter estimation the value of well conductance assigned to a particular well boundary condition will be the value of the well parameter multiplied by the conductance factor. For more information on WEL parameters and conductance factors see the MODFLOW 2000 manual.

Display Cell IDs/IJK

The radio group at the bottom of the dialog allows the user to adjuster whether the cell ID or the cell i, j, k values are displayed for the cells containing the boundary condition/source/sink.

Delete All

The Delete All button deletes all of the data currently defined in the River package and restores the River package parameters to the default values.

6.3.2. MODFLOW Pre-Processing

Building a MODFLOW Model

Two basic approaches are provided in GMS for constructing a MODFLOW model: the model can be completely defined using the tools in the 3D Grid module, or the model can be defined with the aid of the feature objects in the Map module. Also, scatter points and solids can be used to define layer elevation, and boreholes can be used with TPROGS to create material sets for the 3D grid.

Basic Steps in Building a MODFLOW Model

The basic steps in building a MODFLOW model include:

- Build a 3D grid defining the extents of the model. Two approaches are available:
  - MODFLOW Grid Approach
  - MODFLOW Conceptual Model Approach
- Initialize MODFLOW
- Assign boundary conditions and model stresses, including sources and sinks
- Define layer elevations
- Assign material properties
- Run MODFLOW

MODFLOW Array Editor

The MODFLOW Array Editor is used throughout the MODFLOW interface to edit array based data. It includes the following features:

Spreadsheet

The array is displayed in a spreadsheet and each value can be selected and edited. Individual layers in the array are displayed one at a time. The edit fields in the spreadsheet associated with inactive cells are dimmed.

Layers

The edit field in the upper left corner of the dialog is used to switch to a different layer.

Multiplier

The multiplier is a value that can be specified to scale all of the values in the array.

Constant -> Grid

The **Constant -> Grid** button prompts for a single value and assigns the value to all of the cells in the entire array.

Constant -> Layer

The **Constant -> Layer** button prompts for a constant value which is assigned to all of the cells in the currently displayed layer.

3D Data Set -> Grid

The **3D Data Set -> Grid** button brings up the Select Data Set dialog listing all of the current data sets associated with the 3D grid. The selected data set is then copied into the starting heads array. This option is typically used to load in a previously computed MODFLOW solution to use as the initial condition. The previously computed solution must be imported as a data set before selecting this option.

2D Data Set -> Layer

The **2D Data Set -> Layer** button allows the user to select one of the data sets associated with a 2D grid and copy it to the current layer of the starting heads array. In order for this button to be active, a 2D grid that has the same number of rows and columns as the 3D grid must be imported or created. Such a grid can be automatically generated using the ***Grid -> 2D Grid*** command in the *Grid* menu. The 2D Data Set -> Layer option is typically used to load in a data set that has been created by interpolating heads from a 2D scatter point set to the 2D Grid.

Grid -> 3D Data Set

The Grid -> 3D Data Set button copies values from the entire starting heads array to the 3D grid data set list.

Layer -> 2D Data Set

The Layer -> 2D Data Set button copies values from the selected layer of the starting heads array to the 2D grid data set list.

MODFLOW Grid Approach

Building a MODFLOW 3D Grid

For models with simple geometry and boundary conditions, the entire model can be constructed using the tools and commands in the 3D Grid module. With this approach, the editing of the MODFLOW data is performed directly on the grid on a cell-by-cell basis. The main steps are as follows:

- Create a 3D cell-centered grid covering the domain to be modeled using the ***Create Grid*** command in the *Grid* menu.
- Use the commands in the MODFLOW menu to initialize and define the data required by the MODFLOW packages.
- Boundary conditions such as wells are defined by selecting the cells and assigning the attributes directly to the cells.

Defining the Layer Data

An important part of a MODFLOW model is the definition of the layer data (hydraulic conductivity, layer elevations, leakance, etc.). While both the Grid and Map module approaches to constructing a MODFLOW model can be used to define the layer data, both approaches may lead to an overly simplistic definition of the stratigraphy. Layers with spatially varying thicknesses can be handled most effectively using a special set of layer data tools provided in GMS. Solids can also be used to define layer data with the ***Solids->MODFLOW*** and ***Solids->HUF*** commands.

MODFLOW Conceptual Model Approach

A MODFLOW model can be created in GMS using one of two methods: assigning and editing values directly to the cells of a grid (the grid approach), or by constructing a high level representation of the model using feature objects in the Map module and allowing GMS to automatically assign the values to the cells (the conceptual model approach). Except for simple problems, the conceptual model approach is typically the most effective.

Definition

In GMS, the term conceptual model is used in two different ways. In the generic sense, a conceptual model is a simplified representation of the site to be modeled including the model domain, boundary conditions, and material zones. GMS also has a conceptual model object, that can be defined in the Map module. The conceptual model object can contain coverages.

A conceptual model object can be defined in the Map module using feature objects, such as points, arcs, and polygons. The conceptual model is constructed *independently* of the numerical grid. Once the conceptual model object is defined, a grid can be automatically generated to fit the conceptual model. The boundary conditions and model parameters are computed and assigned to the proper cells. The MODFLOW data are converted from the conceptual model to the cells of the grid. This approach to modeling fully automates the majority of the data entry and eliminates the need for most or all of the tedious cell-by-cell editing traditionally associated with MODFLOW modeling. Once the conceptual model is constructed and converted to a grid, the package dialogs and interactive editing tools in the *MODFLOW* menu can be used to edit or review the data if desired.

A complete conceptual model object consists of several coverages. One coverage is typically used to define the sources and sinks such as wells, rivers, lakes, and drains. Another coverage (or the same coverage) is used to define the recharge zones. Other coverages can be used to define the zones of hydraulic conductivity within each layer. Any

number of coverages may be used, or all these attributes may exist in the same coverage.

In addition to the feature data, a conceptual model may include other data (scatter points, boreholes, solids) to define the layer elevations. A specialized set of tools for manipulating layer elevation data is provided in GMS.

Steps in Developing a Conceptual Model

Several steps are involved in setting up a MODFLOW conceptual model and converting the conceptual model to a numerical model. The basic steps are as follows:

1. Create a MODFLOW conceptual model in the Map Module.
2. Decide how many coverages you will need and what attributes you want with each. It is typical to use three coverages, each with a different purpose. One coverage is used for sources and sinks, like wells, specified head boundaries etc. Another coverage is used for recharge, and another is used for hydraulic conductivity. However, it is not required to use coverages in this manner, and the attributes associated with a coverage are user defined, so you can define a coverage with any combination of attributes. Thus, if your recharge zones were the same as your hydraulic conductivity zones, you might use just one coverage for both.
3. Create the sources and sinks. The most effective way to do this is with the aid of a background Image. A digital image representing a scanned map or an aerial photo of the site can be imported and displayed in the background using the image tools. Once the image is displayed, feature objects defining the model boundary, rivers, lakes, flow barriers, and specified head boundaries can be created on top of the background image.
4. Create the areal features, such as recharge zones and evapotranspiration zones.
5. Create the layer features, such as hydraulic conductivity zones.
6. Use the ***Grid Frame*** command to place an outline of the numerical grid on the conceptual model. The frame is placed so that it just surrounds the conceptual model. The frame can be rotated if necessary if the major axis of the model is at an angle.
7. Use the ***Feature Objects | Map -> 3D Grid*** command to automatically generate a grid. The location of the grid is controlled by the Grid Frame and the density of the grid is automatically adjusted around user-specified points (typically wells).
8. Define the active region of the grid using the Activate Cells in Coverage command. This automatically activates all of the cells within the boundary of the conceptual model and inactivates all cells outside the boundary.
9. Initialize the MODFLOW data by selecting the ***New Simulation*** command in the *MODFLOW* menu. Select the type of mode (steady state vs. transient) and define stress periods if necessary. Define a set of starting heads. Go to the LPF/BCF/HUF Package dialog and define the layer type for each of the layers in the grid.
10. Select the ***Map -> MODFLOW*** command to automatically assign the MODFLOW boundary conditions, stresses, and material properties to the appropriate cells in the grid.
11. Use the specialized interpolation tools to define the layer elevations.

In many cases, it is useful to repeat some, but not all, of these steps. For example, suppose after running a simulation it is determined that one of the boundaries of the model corresponding to a groundwater divide is not properly located. The boundary can be moved by simply selecting and dragging the vertices and nodes of the arc(s) defining the boundary. Once the boundary is moved, step 6 should be repeated to redefine the active/inactive regions and then step 8 is repeated to reassign the model data to the cells.

Example Application

To illustrate the conceptual model approach, consider the site shown in the following figure. It represents information that might be available from a combination of sources including maps, photos, and GIS data. This information may include the location of hydrologic features as well as hydrologic properties of the site. However, this information is not yet organized into a form that is useful to a numerical model.

The first step in creating a conceptual model of this site is to create points, arcs and polygons that represent hydrologic features at the site. These points, arcs and polygons are assigned types that correspond to the feature they represent. Based on the attribute type, parameters such as head, concentration and conductance are assigned to these feature objects. The resulting coverage is shown in the following figure. Other coverages, defining such things as recharge zones, would also be defined.

The final step is to take the information that is stored in the conceptual model and construct a numerical model. GMS automates both the creation of the grid geometry as well as assigning boundary conditions and material parameters to the grid. Refine points can be used to specify areas where the grid should have a high density. By specifying polygons that represent the domain of the model, it is possible to automatically inactivate all the cells that lie outside that domain. Boundary conditions may be applied to the individual cells that are intersected by specified feature objects. In addition to determining which cells are assigned boundary conditions, GMS also calculates the appropriate values to assign to each stress period of a transient simulation. The resulting numerical model is illustrated in the following figure.

Advantages of the Conceptual Model Approach

There are numerous benefits to the conceptual model approach. First of all, the model can be defined independently of the grid resolution. The modeler does not need to waste valuable time computing the appropriate conductance to assign to a river cell based on the length of the river reach within the cell. This type of computation is performed automatically. Furthermore, transient parameters such as pumping rates for wells can also be assigned independently of model discretization. Transient parameters are entered as a curve of the stress vs. time. When the conceptual model is converted to the numerical model, the transient values of the stresses are automatically assigned to the appropriate stress periods. Since the conceptual model is defined independently of the spatial and temporal discretization of the numerical model, the conceptual model can be quickly and easily changed and a new numerical model can be generated in seconds. This allows the modeler to evaluate numerous alternative conceptual models in the space of time normally required to evaluate one, resulting in a more accurate and efficient modeling process.

A further advantage of storing attributes with feature objects is that the method of applying the boundary conditions to the grid cells reduces some of the instability that is inherent in finite difference models such as MODFLOW and MT3DMS. When the user enters individual values for heads and elevations, entering cell values one cell at a time can be tedious. It is also difficult to determine the correct elevation along a river segment at each cell that it crosses. The temptation is to select small groups of cells in series and apply the same values to all of the cells in the group. This results in an extreme stair-step condition that can slow or even prevent convergence of the numerical solver. By using GMS to interpolate values at locations along a linear boundary condition such as a river, the user insures that there will be no abrupt changes from cell to cell-thus minimizing the stair-step effect. It also produces a model with boundary conditions that more accurately represent real world conditions.

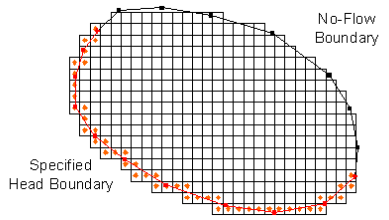
Defining the Layer Data

An important part of a MODFLOW model is the definition of the layer data (hydraulic conductivity, layer elevations, leakance, etc.). While both the Grid and Map module approaches to constructing a MODFLOW model can be used to define the layer data, both approaches may lead to an overly simplistic definition of the stratigraphy. Layers with spatially varying thicknesses can be handled most effectively using a special set of layer data tools provided in GMS. Solids can also be used to define layer data with the ***Solids->MODFLOW*** and ***Solids->HUF*** commands.

Activate Cells in Coverage

Once a grid has been created, the next step in converting a MODFLOW conceptual model to a numerical model is to inactivate the cells which lie outside the boundary of the conceptual model. This is accomplished by selecting the ***Activate Cells in Coverage*** command in the *Feature Objects* menu. When this command is selected, GMS utilizes the polygons in the coverage that is designated as the model boundary to determine which cells should be active and which cells should be inactive. Each cell is compared with the polygons in the coverage and if the cell does not lie within the interior of any of the polygons, the cell is determined to be outside the domain of the model and is inactivated. Cells inside the model domain are made active.

When cells are tested to determine whether they are outside or inside the model domain, if the cell lies partially inside the model domain and partially out, the attribute type of the feature object on the boundary where the cell is located is used to determine the active/inactive status of the cell. An example of this process is shown in the figure at the right.



Sample Application of the Activate Cells in Coverage Command

If an arc on the boundary of the model domain has no attribute assigned to it, it is assumed to be a no-flow boundary. If a cell is partially covered by a no-flow boundary, the cell is activated if the majority of the cell area is inside the coverage. Conversely, the cell is inactivated if the majority of the cell area is outside the coverage. As a result, the outer edges of the cells along the no-flow boundary approximately coincide with the no-flow arc.

If an arc on the boundary of the model domain has a head dependent attribute assigned to it, a different test is used. Any cell that intersects the arc is designated as active, regardless of what percentage of the cell is inside the model domain. As a result, the centers of the cells along the boundary approximately coincide with the source/sink arc. This is appropriate in this case since the stresses are applied in MODFLOW at the cell centers.

Stress Periods

The computational time intervals for a MODFLOW simulation are called "stress periods". The transient stresses (pumping rates, river stages, etc.) can only change at the beginning of each stress period. Stress periods can be subdivided into smaller time steps, if desired. The Stress Periods button in the *Global Options\Basic Package* dialog is used to bring up the *Stress Period* dialog. The stress periods should be defined before any of the sources/sinks are entered. If the steady state option in the *Global Options\Basic Package* dialog is selected, the Stress Periods button is dimmed.

Each stress period is now a single row in the spreadsheet. The stress period properties such as length and number of time steps can now be copied quickly and easily to other stress periods using the spreadsheet interface.

Initialize

A set of stress periods can be defined using the Initialize button. The Initialize button brings up a dialog which is used to generate a set of stress periods of constant length. The dialog prompts for a number of stress periods, a length, a number of time steps, and a time step multiplier. A set of stress periods is then generated and displayed graphically in the stress period plot.

Stress Period Plot

The horizontal strip at the top of the Stress Periods dialog is used to graphically edit stress periods. A stress period can be selected in the plot by clicking on the stress period with the mouse. The values associated with the selected stress period can be edited in the spreadsheet.

Insert Buttons

New stress periods can be added by selecting a stress period and selecting either the Insert Row button  or by editing the last row in the spreadsheet. Stress periods can be deleted by selecting the stress periods and selecting the Remove Row button  .

Reference Time

The first cell in the spreadsheet is used to enter the reference time for the MODFLOW simulation. The reference time is the date/time corresponding to the beginning of the simulation (t=0). If the Use Date/Times option is selected in the Time display section, all time values entered for transient input data, i.e., time series defined in the XY Series Editor can be entered in a date/time format rather than a scalar time format. Also, when post-processing, the values shown in the time step selector in the Data Browser or at the top of the GMS Window are displayed in the date/time format. Furthermore, any time series curves entered as part of the MODFLOW conceptual model in the Map module that were defined using the date/time format will be automatically converted to the proper time scale when the conceptual model is converted to grid-based numerical model.

Map to MODFLOW

After the conceptual model is constructed and a grid has been created, the final step in converting a conceptual model to a MODFLOW numerical model is to select the Map -> MODFLOW command. However, before this command can be selected, MODFLOW must be initialized. MODFLOW is initialized as follows:

1. Switch to the 3D Grid module
2. Select the ***New Simulation*** command in the *MODFLOW* menu.
3. MODFLOW simulations are steady state by default. For a transient simulation, go to the *Global Options/Basic Package* Dialog and select the **Transient** option. Then set up the stress periods you wish to use in the simulation.
4. By default, the top layer is unconfined and the remaining layers are confined. To use a different set of layer types, go to the BCF/LPF/HUF Package dialog and select the appropriate layer type for each layer.

Once MODFLOW is initialized, the ***Map -> MODFLOW*** command becomes available. When the command is selected, the *Map -> MODFLOW Options* dialog appears. Three options are available for converting the conceptual model: Active coverage only, All applicable coverages, and All visible coverages. If the All applicable coverages option is chosen, all of the feature objects in all of the MODFLOW-related coverages in the active conceptual model are used. This option is typically selected when the conceptual model is first converted. If the Active coverage only or the All visible coverages option is selected, only a subset of the coverages are used to update the numerical model.

Temporal Discretization

See the Temporal Discretization page.

Multiple Values Per Cell

Because GMS processes each feature object separately, there will often be sources/sinks that were derived from two separate feature objects in the same cell. In fact, this is almost always the case in the cell that contains the endpoint of one arc and the beginning point of an adjacent arc. This is not an error. MODFLOW handles each of the boundary conditions in the cell simultaneously.

Specified Head Cells

Because the constant head condition forces the head in those cells to match whatever is specified, it is inappropriate to have other boundary conditions defined in the cells that are designated constant head. Therefore, GMS processes all of the specified head objects first. Afterwards, if there is another stress that should normally be assigned to a cell that has been previously assigned a constant head condition, the new stress is not assigned.

Changing Head Boundary

When mapping a specified head boundary to MODFLOW, GMS always uses the CHD package (Time Variant Specified Head package). In MF2K, a changing head boundary must be used in order to extract fluxes out of the MODFLOW output for the arcs in the map module. With MF2K you can not get a flux observation with normal Spec Head. It is assumed that most of the time the user would want to see the flux in/out of the boundary. If a cell contains two different arcs, the specified head is split in 2 pieces at cells where 2 specified head arcs meet. This is done for 2 reasons. First, the CHD package will combine the CHD boundary conditions that are in the same cell. Second, the flux in/out of the cell will be partitioned to the 2 different arcs in the map module.

A traditional specified head boundary can be manually applied by using the IBOUND and starting heads arrays. The computed heads from MODFLOW will be the same whether a constant head or changing head boundary is used.

Well Screens

NOTE: This approach was developed prior to the existance of the MNW package. The MNW package can more accurately represent a well that crosses multiple MODFLOW layers.

When using well screens in your conceptual model the following equation is used to partition the flow to different layers:

$$Q_i = \frac{T_i}{T} = \frac{(k_h)_i B_i}{\sum_{j=1}^{n} (k_h)_i B_i}$$

where

Q_i = The flow rate for layer i

$(kh)_i$ = The horizontal hydraulic conductivity for layer i

B_i = The length of the well screen intercepted by the layer

For example

Assuming the K's are the horizontal K's, Q_1 would be computed as:

$$Q_1 = \frac{K_1 B_1}{K_1 B_1 + K_2 B_2 + K_3 B_3}$$

In order to complete this computation, the K's must be assigned to the cells in the grid. You must assign the K values to the grid prior to executing the ***Map -> MODFLOW*** command.

If the HUF package is being used then the K value for each cell is estimated from the HUF units.

Automatic Layer Assignment

When building a MODFLOW conceptual model with a multi-layer model, it is necessary to define the range of layers associated with a particular source sink object. For example, an arc corresponding to a specified head boundary condition may be associated with layers 1-3 on the edge of a model. On the other hand, a drain arc in the middle of the model may only be associated with the top layer. The following example shows how a specified head boundary condition would map with the "Use layer range" option with the range set from 1 to 2:

In some cases, however, the proper layer for a particular source/sink object will depend on the elevation of the object relative to the layer elevations. For example, a drain may represent a channel that cuts through the terrain. In some places the channel may be shallow and correspond to layer 1. In other places, the channel may be deep enough that it cuts into layer 2. The "Auto assign to one cell" option is used for defining the layer range in these cases. If this option is selected, the object will be associated with the layer where the elevation or head associated with the object falls between the top and bottom elevation for the layer. The following shows how the same specified head boundary condition would map with the "Auto assign to one cell" option:

The "Auto-assign including lower cells" option is useful for cases where you want a specified head boundary assigned to the layer where the head is between the top and bottom elevation of the cell as well as any active cells below that cell. The following shows how the same specified head boundary condition would map with the "Auto-assign including lower cells" options:

Using TINs

TIN surfaces can be used as part of the conceptual model. See the Map to MODFLOW with TINs page.

Defining the Layer Elevations

One of the most important steps in defining a MODFLOW model is to define the layer elevations. The layer elevations are stored in the *Global Options/Basic package*. The layer elevations include a top elevation for layer 1 and a bottom elevation for all layers. For all layers except for the top layers, the top elevation for the layer is assumed to be equal to the bottom elevation of the layer above.

Define Layer Data

As described above, MODFLOW models can be defined using one of two approaches: (1) by editing the input values on a cell-by-cell basis directly on the grid, or (2) by creating a high level conceptual model using the Map module. Both approaches can be used to define the layer elevation arrays. With the grid approach, a constant value can be assigned to the entire array at once or to a set of selected cells. With the conceptual model approach, a set of polygons can be used to define zones of elevations within each layer. While these two approaches are simple to use, in most cases they result in an overly simplistic stair step definition of the layer elevations. In most cases, it is more appropriate to use the 2D geostatistical tools in GMS to smoothly interpolate layer elevations.

Interpolating Elevation Data

The following steps are used to interpolate elevation data:

Step 1 - Importing the Scatter Point Elevation Data

The fist step in defining MODFLOW layer elevation array data is to create a 2D scatter point set. The set should include a data set for the top elevation of the top layer and the bottom elevation array of the top layer and each of the underlying layers. A water table elevation corresponding to the desired initial condition (starting head) may also be defined. The simplest way to create such a scatter point set is to create a tabular scatter point file using a spreadsheet or a text editor. The scatter point file is imported ***File\Open*** menu command. A sample tabular scatter point file for a three layer model is shown below:

x	y	top1	bot1	bot2	bot3
360	1670	450	345	200	100
290	870	445	340	195	95
480	420	450	350	200	100
620	2120	455	245	200	100
990	1820	470	355	210	115
890	1190	465	350	205	110
1030	710	475	360	215	130
etc.					

Step 2 - Interpolating the Elevations to the MODFLOW Arrays

Once the scatter point file is imported to GMS, the next step in defining MODFLOW layer elevation arrays is to interpolate the elevations to the MODFLOW layer elevation arrays. The elevation values can be interpolated directly to the MODFLOW arrays using the ***...to MODFLOW Layers*** command in the *Interpolation* menu in the 2D Scatter Point module. When this command is selected, the Interpolate to MODFLOW Layers dialog appears.

The purpose of this dialog is to associate each of the data sets in the scatter point set with one of the layer data input arrays. A data set and the corresponding layer data array are selected in the top of the dialog and the Map button is selected. The defined relationship is then shown in the bottom of the dialog. Once this is completed for each data set/layer data array combination, the **OK** button is selected and the scatter point data set values are interpolated directly to the MODFLOW arrays using the currently selected interpolation options.

In some cases, GMS can automatically match the scatter point data sets to the appropriate layer elevation arrays. GMS searches each data set name to see if "top" or "bot" makes up any portion of the name. If so, it then searches for a number to determine the layer the array should be interpolated to. For example, the data set names top1, top of layer 1, and top elevation of layer 1 would all automatically map correctly.

It should be noted that the layer data can be set up using multiple scatter point sets. For example, it is possible to have one dense set of scatter points to define the ground surface (top of layer one), and a second, more sparse set of scatter points to define the layer bottom elevations. In this case, the to Layers command would need to be selected twice, once for each of the scatter point sets.

Step 3 - Fixing Layer Interpolation Errors

When interpolating layer data for the purpose of defining MODFLOW layer elevation arrays, there are often cases where the interpolated values overlap. For example, for some of the cells, the top elevation values for a particular layer may be lower than the bottom values for the layer. In some cases, the best way to fix such a problem is to experiment with the interpolation options or to create some "pseudo-points" to fill in the gaps between sparse scatter points. In other cases, the overlap may correspond to a pinchout or truncation in the layer. In such cases, the elevations need to be adjusted so that there is a small but finite thickness for all cells in the overlapping region.

The first step in fixing layer errors is to use the Model Checker to determine if elevation overlaps occur. If they do occur, the Fix Layer Errors button at the top of the Model Checker dialog can be used to bring up the *Fix Layer Errors* dialog. The number of overlap errors for each layer is listed on the right side of the dialog. A layer is highlighted and a correction method is selected on the left side of the dialog. The **Fix Selected Layer** button is then used to adjust the elevations. Four options are available for fixing layer errors:

Average

With the Average method, for each cell where an overlap is found, the average elevation at the overlap is computed as

$$\text{ave} = \frac{\text{top} - \text{bottom}}{2}$$

The top and bottom elevations are then adjusted as follows:

$$\text{top} = \text{ave} + \frac{\text{min thickness}}{2}$$

$$\text{bot} = \text{ave} - \frac{\text{min thickness}}{2}$$

This option is useful for modeling the transition zones adjacent to embedded seams.

Preserve Top

With the Preserve top method, at each cell, where an overlap is found the top elevation is unchanged and the bottom elevation is adjusted to:

$$\text{bot} = \text{top} - \text{min thickness}$$

This option can be used to model truncated outcroppings.

Preserve Bottom

With the Preserve bottom method, at each cell where an overlap is found the bottom elevation is unchanged and the top elevation is adjusted to:

$$\text{top} = \text{bot} + \text{min thickness}$$

Truncate to Bedrock

The Truncate to bedrock option differs from the other methods in that it can be used to alter several layers at once. With this method, it is assumed that the bottom elevation values for the bottom layer represent the top of a bedrock unit. The bedrock elevations may overlap several upper elevation arrays. Each cell in the grid is checked and if the bedrock elevation is above the top elevation for the cell, the cell is turned off (made inactive). If the bedrock elevation is below the top elevation and above the bottom elevation for the cell, the bottom elevation for the cell is set equal to the bedrock elevation. If the bedrock elevation is below the bottom of the cell, the cell elevations are unchanged.

Define Layer Data with Solids

Solids can also be used to define layer data for MODFLOW. The ***Solids -> MODFLOW*** and ***Solids -> HUF*** commands in the Solid module set up the layer elevations using the currently defined solids.

Standard MODFLOW Parameters

Caution

There are two ways to do MODFLOW parameterization in GMS:

1. The key value method **(recommended)**
2. The standard MODFLOW method

The "key value" approach is the preferred approach to defining parameters in GMS. Using key values is the only option for WEL, RIV, DRT, DRN, GHB, CHD, STR, and HFB parameters. In GMS, using the key value approach with these parameters provides the same functionality of parameter instances available in MODFLOW.

Key values can also be used with array based parameters. However, GMS does support defining array based parameters with clusters and instances (for ETS, EVT, RCH parameters).

When reading in a MODFLOW simulation that was created outside of GMS all parameters will be converted to key values so long as the parameter can be represented by key values.

Key values can not be used to represent an array based parameter if the parameter is defined using more than one cluster or more than one instance. Also, if more than one parameter uses the same zone array with a matching IZ value then the parameter can not be represented using key values. Further, if the multiplier array associated with the parameter has values other than 1.0 in the zones where the parameter is used then the parameter can not be represented with key values.

The standard MODFLOW method is considered an "advanced" feature in GMS. **Only users that understand how MODFLOW uses parameters should attempt to use this feature.**

This article describes how to use the standard MODFLOW parameterization method in GMS.

Support in GMS

Reading

GMS can read MODFLOW models that use standard MODFLOW parameters.

Writing

GMS writes MODFLOW models using the key value approach. So, although GMS can read models that use standard MODFLOW parameters, it cannot write them using the standard MODFLOW parameter method. Writing is usually done using the key value method. There are a few exceptions which include recharge and evapotranspiration parameter instances, and LPF and HUF parameter clusters. GMS will write these parameters using the standard MODFLOW parameter method because these cannot always be represented using the key value method.

Editing

When GMS reads a model that uses standard MODFLOW parameters it converts them to regular GMS key value approach parameters. The parameters can then be edited using the *Parameters* Dialog. Recharge, evapotranspiration, LPF, and HUF parameters are special in that you can edit the instance and cluster information associated with these types of parameters.

MODFLOW Parameter Clusters Dialog

The *MODFLOW Parameter Clusters* Dialog allows users to define instances for RCH, EVT, LPF, and HUF parameters that use clusters. The inputs in this dialog basically follow the necessary inputs for defining a parameter instance in a package file. You may wish to review the MODFLOW Parameter Clusters and Instances section below.

Array based parameters are defined using clusters. A cluster is a multiplier array, a zone array, and specified zone values where the parameter is applied. Multiplier arrays and zone arrays have associated datasets underneath the three dimensional grid in the Project Explorer.

Instances are enabled for RCH and EVT parameters. Instances allow the user to define multiple sets of clusters that are all tied to one parameter. Then the user may use different instances in different stress periods in their MODFLOW model. For more information on parameter instances consult the MODFLOW documentation.

In the MODFLOW Parameters dialog the user selects the **Define clusters** option for a parameter. This will allow the user to specify the number of instances and clusters that are used to define the parameter.

In the *Parameter Instances* dialog the user defines a name for each parameter instance for RCH and EVT parameters. For LPF parameters a level is defined and for HUF parameters a hyrdogeologic unit is defined. Then for each cluster the user selects a multiplier array and a zone array. These are datasets on the 3D Grid. The user must also specify the zone values (IZ) where the parameter is to be applied in the model. If there is more than one IZ value for the cluster then the user enters the numbers with spaces between the entries. So if the parameter is to be applied where the zone array values are 1 and 3 then the user would enter "1 3". The user must also specify the stress periods where an instance is to be used. The numbers entered in the Stress Periods field should also be space delimited. This means if you want an instance to be used in stress periods 1, 2, and 5 then your entry in the Stress Periods field should be "1 2 5".

When the package is written out for MODFLOW the instances will be included in the parameter definition and used for forward runs or for parameter estimation runs.

MODFLOW Parameter Clusters and Instances

For those wanting to follow the standard MODFLOW approach to parameterization, the following explanation may be helpful. You should refer to the MODFLOW documentation for more information.

Definitions

Here is a brief review of the most important terms used when dealing with parameters.

- *Parameter* – Has a name, type, one or more clusters, and zero or more instances.
- *Parval* – The value of the parameter.
- *Cluster* – Has a multiplier array (*Mltarr*), a zone array (*Zonarr*), and zone numbers (*IZ*).
- *Mltarr* – Name of the multiplier array. Parval is multiplied by this to define the value.
- *Zonarr* – Name of the zone array used to define the cells that are associated with a parameter.
- *IZ* – Up to 10 zone numbers (separated by spaces) that define the cells that are associated with a parameter.
- *Instance* – Parameter cluster that could be used for different stress periods in a MODFLOW simulation.

Examples

Below are some examples showing different ways parameters can be used. The examples use parameters to define recharge for a forward run (not doing inverse modeling). The grid in the examples is 5 rows, 5 columns, 1 layer. The examples use the following multiplier and zone arrays.

Multiplier arrays

MULT0001

1.0	1.0	1.0	1.0	1.0
1.0	1.0	1.0	1.0	1.0
1.0	1.0	1.0	1.0	1.0
1.0	1.0	1.0	1.0	1.0
1.0	1.0	1.0	1.0	1.0

MULT0002

0.5	0.5	0.5	0.5	0.5
0.5	0.5	0.5	0.5	0.5
0.5	0.5	0.5	0.5	0.5
0.5	0.5	0.5	0.5	0.5
0.5	0.5	0.5	0.5	0.5

Zone Arrays

ZONE0001

2	2	2	0	0
2	2	2	0	0
2	2	2	0	0
0	0	0	0	0
0	0	0	0	0

ZONE0002

3	3	3	3	3
3	3	3	3	3
4	4	4	4	4
4	4	4	4	4
5	5	5	5	5

ZONE0003

0	0	0	0	0
0	0	6	7	0
0	0	6	7	0
0	0	0	0	0
0	0	0	0	0

Example 1

Steady state. 1 recharge parameter with 1 cluster, 1 instance.

Recharge file	Variables	Explanations
`PARAMETER 1`	`PARAMETER NPRCH`	`One recharge parameter will be used`
`3 40`	`NRCHOP IRCHCB`	`Apply to highest active cell, save CCF to unit 40`
`Param1 RCH 0.00005 1`	`PARNAM PARTYP Parval NCLU`	`Parameter name, type, value and number of clusters`
`MULT0001 ZONE0001 2`	`Mltarr Zonarr IZ`	`Multiplier array, zone array, and zone number`
`1 1`	`INRECH INIRCH`	`One parameter used in current stress period, INIRCH (ignored)`
`Param1`	`Pname`	`Name of parameter used to define RECH in this stress period`

Results

The resulting recharge applied to the top-most active layer would be:

0.00005	0.00005	0.00005	0	0
0.00005	0.00005	0.00005	0	0
0.00005	0.00005	0.00005	0	0
0	0	0	0	0
0	0	0	0	0

Example 2

Steady state. 2 recharge parameters:

- the first with 1 cluster, 1 instance
- the second with 2 clusters, 1 instance.

Recharge file	Variables	Explanations
PARAMETER 2	PARAMETER NPRCH	Two recharge parameters will be used
3 40	NRCHOP IRCHCB	Apply to highest active cell, save CCF to unit 40
Param1 RCH 0.00005 1	PARNAM PARTYP Parval NCLU	Parameter name, type, value and number of clusters
MULT0001 ZONE0001 2	Mltarr Zonarr IZ	Multiplier array, zone array, and zone number
Param2 RCH 0.00004 2	PARNAM PARTYP Parval NCLU	Parameter name, type, value and number of clusters
MULT0002 ZONE0002 4 5	Mltarr Zonarr IZ	Multiplier array, zone array, and zone numbers
MULT0002 ZONE0003 6 7	Mltarr Zonarr IZ	Multiplier array, zone array, and zone numbers
2 1	INRECH INIRCH	Two parameters used in current stress period, INIRCH (ignored)
Param1	Pname	Name of parameter used to define RECH in this stress period
Param2	Pname	Name of parameter used to define RECH in this stress period

Results

The intermediate results for each parameter cluster are listed below:

Param1

0.00005	0.00005	0.00005	0	0
0.00005	0.00005	0.00005	0	0
0.00005	0.00005	0.00005	0	0
0	0	0	0	0
0	0	0	0	0

Param2, cluster 1

0	0	0	0	0
0	0	0	0	0
0.00002	0.00002	0.00002	0.00002	0.00002
0.00002	0.00002	0.00002	0.00002	0.00002
0.00002	0.00002	0.00002	0.00002	0.00002

Param2, cluster 2

0	0	0	0	0
0	0	0.00002	0.00002	0
0	0	0.00002	0.00002	0
0	0	0	0	0
0	0	0	0	0

The final result after accumulating each cluster is:

0.00005	0.00005	0.00005	0	0
0.00005	0.00005	0.00007	0.00002	0
0.00007	0.00007	0.00009	0.00004	0.00002
0.00002	0.00002	0.00002	0.00002	0.00002
0.00002	0.00002	0.00002	0.00002	0.00002

Example 3

Transient. 1 recharge parameter with 1 cluster, 2 instances. One instance is used in the first and third stress periods, and the other is used in the second stress period.

Recharge file	Variables	Explanations
PARAMETER 1	PARAMETER NPRCH	One recharge parameters will be used
3 40	NRCHOP IRCHCB	Apply to highest active cell, save CCF to unit 40
Param1 RCH 0.00005 1 INSTANCES 2	PARNAM PARTYP Parval NCLU INSTANCES NUMINST	Parameter name, type, value number of clusters, number of instances
Instance1	INSTNAM	Instance name
MULT0001 ZONE0001 2	Mltarr Zonarr IZ	Multiplier array, zone array, and zone number
Instance2	INSTNAM	Instance name
MULT0002 ZONE0001 2	Mltarr Zonarr IZ	Multiplier array, zone array, and zone number
1 1	INRECH INIRCH	One parameters used in current stress period, INIRCH (ignored)
Param1 Instance1	Pname Iname	Name of parameter and name of instance used in this stress period
1 1	INRECH INIRCH	One parameters used in current stress period, INIRCH (ignored)
Param1 Instance2	Pname Iname	Name of parameter and name of instance used in this stress period
1 1	INRECH INIRCH	One parameters used in current stress period, INIRCH (ignored)
Param1 Instance1	Pname Iname	Name of parameter and name of instance used in this stress period

Results

The intermediate results for each parameter cluster are listed below:

Stress Period 1, Param1, Instance RCH_1_1

0.00005	0.00005	0.00005	0	0
0.00005	0.00005	0.00005	0	0
0.00005	0.00005	0.00005	0	0
0	0	0	0	0
0	0	0	0	0

Stress Period 2, Param1, Instance RCH_1_2

0.000025	0.000025	0.000025	0	0
0.000025	0.000025	0.000025	0	0
0.000025	0.000025	0.000025	0	0
0	0	0	0	0
0	0	0	0	0

Stress Period 3, Param1, Instance RCH_1_1

0.00005	0.00005	0.00005	0	0
0.00005	0.00005	0.00005	0	0
0.00005	0.00005	0.00005	0	0
0	0	0	0	0
0	0	0	0	0

MODFLOW Parameters - Two Methods

Caution

There are two ways to do MODFLOW parameterization in GMS:

1. The key value method **(recommended)**
2. The standard MODFLOW method

The "key value" approach is the preferred approach to defining parameters in GMS. Using key values is the only option for WEL, RIV, DRT, DRN, GHB, CHD, STR, and HFB parameters. In GMS, using the key value approach with these parameters provides the same functionality of parameter instances available in MODFLOW.

Key values can also be used with array based parameters. However, GMS does support defining array based parameters with clusters and instances (for ETS, EVT, RCH parameters).

When reading in a MODFLOW simulation that was created outside of GMS all parameters will be converted to key values so long as the parameter can be represented by key values.

Key values can not be used to represent an array based parameter if the parameter is defined using more than one cluster or more than one instance. Also, if more than one parameter uses the same zone array with a matching IZ value then the parameter can not be represented using key values. Further, if the multiplier array associated with the parameter has values other than 1.0 in the zones where the parameter is used then the parameter can not be represented with key values.

The standard MODFLOW method is considered an "advanced" feature in GMS. **Only users that understand how MODFLOW uses parameters should attempt to use this feature.**

Conductance

Many MODFLOW boundary condition types (i.e., general head, rivers, streams, drains) include a conductance parameter. MODFLOW uses the conductance to determine the amount of water that flows in or out of the model due to the boundary condition stresses.

When using a conceptual model, the manner in which the conductance term should be computed and entered depends on whether the feature object is a polygon, arc or point. Before explaining this fully, a short review of the definition of conductance is appropriate.

Conductance formulation

Darcy's law states:

$$Q = kiA$$

where:

Q = flow rate [L^3/T]

k = hydraulic conductivity [L/T]

i = hydraulic gradient (unitless)

A = gross cross-sectional area of flow [L^2].

Darcy's law can also be expressed as:

$$Q = k\frac{\Delta H}{L}A$$

where:

ΔH = the head loss [L]

L = the length of flow [L]

Since the unknown on the right side is the head, it is convenient to group all of the other terms together and call them conductance:

$$Q = C\Delta H$$

where:

C = conductance [L^2/T]

This results in the following general definition for conductance:

$$C = \frac{k}{L}A$$

This may be represented more specifically in the following form.

$$C = \frac{k}{t}lw$$

where:

t = the thickness of the material in the direction of flow [L]

lw = the cross-sectional area perpendicular to the flow direction [L^2].

Conductance in conceptual models

In the case of a river boundary condition, the conductance is defined in MODFLOW as the hydraulic conductivity of the river bed materials divided by the vertical thickness (length of travel based on vertical flow) of the river bed materials, multiplied by the area (width times the length) of the river in the cell. The last term, area, is the hardest parameter to determine by hand since it varies from cell to cell.

Arcs

Fortunately, GMS can automatically calculate the lengths of arcs and areas of polygons. Therefore, when a conductance is entered for an arc, it should be entered in terms of **conductance per unit length**. For example, in the case of rivers, conductance should be entered as:

$$C_{arc} = \frac{\frac{k}{t}lw}{L} = \frac{k}{t}w$$

where:

Carc = conductance per unit length [(L^2/T)/L] or [L/T]

t = the thickness of the material [L]

w = the width of the material along the length of the arc [L]

When GMS applies the boundary condition from the arc to the grid cell, it automatically multiplies the entered value of conductance by the length of the arc that intersects the cell to create an accurate conductance value for the cell.

Polygons

For polygons, conductance should be entered in a **conductance per unit area** form:

$$C_{poly} = \frac{\frac{k}{t} lw}{A} = \frac{k}{t}$$

where:

Cpoly = conductance per unit area [(L^2/T)/L^2] or [1/T]

t = the thickness of the material [L]

When GMS converts the stress from a polygon to a grid cell, it automatically multiplies the entered value of conductance by the area of the cell that is covered by the polygon to create an appropriate conductance value for the cell. This restores the dimensional accuracy to the expression for conductance.

Points

When a general head, river, stream or drain attribute is assigned to an individual point, the conductance should be entered as a normal conductance value. This conductance is then directly assigned to the cell containing the point.

Parameter Factors

Beginning with GMS version 7.0, the Well, Drain, River, General head, and Stream boundary conditions have a parameter factor field that is associated with each boundary condition. The parameter factor is used with the parameter value to compute the final value of conductance for a given boundary condition (or in the case of the well package the final Q value). The parameter factor is automatically set by GMS when doing the ***Map->MODFLOW*** command. This value will be set to the length of the arc in the cell or the area of the polygon in the cell associated with the boundary condition; for a point feature the factor is set to 1.0.

MODFLOW Parameters Disclaimer

The "key value" approach is the preferred approach to defining parameters in GMS. Using key values is the only option for WEL, RIV, DRT, DRN, GHB, CHD, STR, and HFB parameters. In GMS, using the key value approach with these parameters provides the same functionality of parameter instances available in MODFLOW.

Key values can also be used with array based parameters. However, GMS does support defining array based parameters with clusters and instances (for ETS, EVT, RCH parameters).

When reading in a MODFLOW simulation that was created outside of GMS all parameters will be converted to key values so long as the parameter can be represented by key values.

Key values can not be used to represent an array based parameter if the parameter is defined using more than one cluster or more than one instance. Also, if more than one parameter uses the same zone array with a matching IZ value then the parameter can not be represented using key values. Further, if the multiplier array associated with the parameter has values other than 1.0 in the zones where the parameter is used then the parameter can not be represented with key values.

The standard MODFLOW method is considered an "advanced" feature in GMS. **Only users that understand how MODFLOW uses parameters should attempt to use this feature.**

Saving and Reading a MODFLOW Simulation

Saving a MODFLOW Simulation

Once a MODFLOW simulation has been created and checked for potential problems with the Model Checker, the next step is to save the simulation to disk and run MODFLOW. MODFLOW simulations are saved using the ***Save*** and ***Save As*** commands in the *File* menu.

Selecting the ***Save*** command saves the GMS project including the model simulation. By default the model simulation will be saved to the same location as the GMS project. However, in the Save dialog the path for the model simulation can be specified.

A MODFLOW simulation is actually saved to a set of input files. The MODFLOW super file is used to store extra data used by GMS but not used by MODFLOW. The super file also contains the path to the name file. The names of all of the input and output files associated with a simulation are saved in the name file. When MODFLOW is launched, the name of the super file is automatically passed to the MODFLOW executable.

When a MODFLOW simulation is saved, the names of the other MODFLOW input files are automatically patterned after the name of the super file. For example, if the super file is named sampmod.mfs, the other files are named sampmod.bas, sampmod.bcf, etc.

The user can adjust the output options in the *Output Control* dialog

The version of MODFLOW 2000 that ships with the GMS software has been modified to be able to read and write input data stored in HDF5 files. For more information see MODFLOW with HDF5.

Reading a MODFLOW Simulation

Once a MODFLOW simulation has been saved by GMS using the ***Save*** command in *File* menu, the entire simulation can be read back into GMS using the ***Open*** command in the *File* menu.

MODFLOW simulations can be read in individually (*.mfs) or as part of a project (*.gpr). They can also be imported by using the MODFLOW name file. The extension for the name file must be changed to *.mfn.

Reading a Completed MODFLOW Solution

When you are using the Model Wrapper to control your MODFLOW run, you can use the **Read MODFLOW solution** toggle at the bottom of the dialog to automatically read in the corresponding solution.

You can also read in solution files generated by MODFLOW using the ***Read Solution*** command in the *MODFLOW* menu. This command brings up the a file browser and prompts you to choose a MODFLOW super file (pre GMS 7.0) or a MODFLOW name file (GMS 7.0+).

Output Control

The Output Control dialog is accessed from the *MODFLOW* menu. The Output Control dialog contains the following options:

Output Interval Options

The Output Interval section lets you choose which files you want to output and when you want to output the results. By default, GMS instructs MODFLOW to output heads and volume data to both data files and text output files. Drawdown is not output by default.

Global Output File

Choose this option to use the global output file (*.glo). This file contains information about the input files and, during an inverse run using the PES process, will contain information about each iteration. Either the global file, list file, or both must be used with MODFLOW.

List Output File

Choose this option to use the list output file (*.out). This file contains information about the current MODFLOW run. This file will be overwritten during an inverse run using the PES process for each inverse iteration.

*.hff File For Transport

Select this option to output the head and flow file (*.hff) used by MT3DMS to generate the flow fields for transport modeling.

Save Arrays Using Binary Files

Choose this option to save all 2D arrays used as MODFLOW input as binary arrays in external files. If this option is not selected, the 2D arrays are written within the respective files in ASCII format. The binary option results in more files, but uses less disk space. There is also a time savings during running for MODFLOW models with large grids.

Enable saving of computed flows for all source/sink objects

This option allows GMS to create a flow observation for all sources/sinks that were created using the ***Map->MODFLOW*** command so that the user can see the computed flux through the group of boundary conditions. If the user is doing a transient simulation then having this option may cause MODFLOW to crash because MODFLOW attempts to allocate more memory than any of us have available. Turning off this option in this situation is the best course of action.

Importing MODFLOW Files

GMS imports standard MODFLOW 88, 96, 2000, 2005[1], and MODFLOW-NWT[2] files. GMS supports saving of MODFLOW 2000, 2005, and MODFLOW-NWT so other versions will be converted to MODFLOW 2000, 2005, or NWT.

If GMS created the MODFLOW simulation then you should open the corresponding GMS project file (*.gpr). If there is no GMS project file, you can import the MODFLOW simulation into GMS as described below. GMS will create a new copy of the imported MODFLOW simulation in its own modified MODFLOW file format. Click here for more information on the modified MODFLOW file format.

Native MODFLOW files (ascii/text) can be exported from GMS. Click here for more information on exporting MODFLOW files.

How to import a MODFLOW model into GMS

You can follow these steps when importing a MODFLOW simulation into GMS.

1. Were the MODFLOW files created by GMS?
   - Yes

     If the files were created by GMS, and you have the GMS project file (.gpr), you should just read that into GMS using the standard ***File\|Open*** command. If you don't have the .gpr file, you should import the MODFLOW model into GMS by opening the "super file" (*.mfs) using the standard ***File\|Open*** command. The super file is a non-standard file that GMS creates along with the standard MODFLOW files. If you don't have a super file, proceed to step 2 below.
   - No

     Proceed to step 2 below.
   - Don't know

     If you have a *.gpr file or a *.mfs file, then it's almost certain that the files were created by GMS. If you don't have these files, proceed to step 2 below.
2. Determine whether your model is MODFLOW 88, 96 or 2000. If you are unsure, refer to the section below entitled Determining the MODFLOW version which describes each one.
   - MODFLOW 88

     Read the basic package file into GMS (using the standard *File\|Open* dialog). GMS will attempt to import all the other files.
   - MODFLOW 96

     Read the name file.
   - MODFLOW 2000

     Read the name file.
   - MODFLOW 2005

Read the name file.

- MODFLOW-NWT

  Read the name file.

Troubleshooting

If you are having trouble reading the files into GMS, first verify that MODFLOW can read the files by launching MODFLOW at a command prompt and giving it the name of the file to read. If MODFLOW can read the files but GMS cannot, it may be because you are attempting to import packages which GMS does not support; see MODFLOW Packages Supported in GMS for more information.

Contact tech support [3] for additional help.

Determining the MODFLOW version

MODFLOW 88

To tell if a file is MODFLOW 88 open up the basic package file as a text file. GMS uses *.bas as the extension for this file. The file should appear something like the figure below.

```
Heading 1
Heading 2
          3         23         17          1          4
 11 13 14 15  0  0 16  0  0  0  0 10 12  0  0  0  0  0  0  0  0 29  0  0
          0          0
          1          1               (17I3)          0
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
```

For a MODFLOW 88 file the third line of the basic package file will include an IUNIT array with 24 slots. There may also be an IUNIT array with only 12 slots, if so just ok the warning GMS gives. These slots include the unit numbers for packages included in the file. Every number must be unique to its package. If the number does not correspond to a file then the file is an external array which must be matched by the user. If the basic package file includes an IUNIT array as described it is a MODFLOW 88 file.

To import the MODFLOW 88 file locate the *.mfs file. If there is no *.mfs file then select the *.bas file. Then simply use the ***File|Open*** command to read the file into GMS.

More about MODFLOW 88 files

MODFLOW 88 files have no name (*.nam or *.mfn) file.

GMS makes a few assumptions when reading in MODFLOW 88 files:

1. All files must have the same prefix.
   - Example: If the files are named bas.dat, drain.dat, and river.dat they all must be converted to run1.bas, run1.drn, and run1.riv
2. All files use the standard GMS suffixes as shown in the table below.
   - If these are not the suffixes in use, you will need to rename the files.
3. IUNIT slots must be standard with standard ID #'s according to MODFLOW documentation.

4. It is up to the user to know what external arrays go to which MODFLOW files. Otherwise the files will not be properly read in.
    - GMS can import external arrays but is unable to import external binary arrays
5. MODFLOW 88 files use a fixed format.

MODFLOW 88 IUNIT Array Positions and Packages

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
BCF	WEL	DRN	RIV	EVT		GHB	RCH	SIP	DE4	SOR	OC	PCG	GFD		HFB	RES	STR	IBS	CHD

Standard GMS Extensions for MODFLOW 88 files

Package	Extension
BASIC	*.bas
OUTPUT CONTROL	*.oc
BCF	*.bcf
RIVER	*.riv
DRAIN	*.drn
WELL	*.wel
GENERAL HEAD BOUNDARY	*.ghb
STREAM	*.str
RECHARGE	*.rch
EVAPOTRANSPIRATION	*.evt
STRONGLY IMPLICIT PROCEDURE	*.sip
SLICE-SUCCESSIVE OVERRELAXATION	*.sor

MODFLOW 96

To tell if model files are in MODFLOW 96 format, open up the basic package file as a text file. For a MODFLOW 96 file the third line of the *.bas file will NOT include an IUNIT array. Instead the third line will say FREE, which means that the data in the file is in free format and each data entry is separated with a space. A 96 file may not contain the FREE line. Instead the line may be blank and the file may be fixed format. This file can be read in just the same using the name file.

```
Heading 1
Heading 2
         3         23         17          1          4
FREE
          0          0
INTERNAL 1 (free) 0 "Ibound Layer 1"
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

If the basic package file says FREE as described it is a MODFLOW 96 file. A name file (typically with a *.mfn or *.nam extension) should also exist. If one does not it must be created as described below.

To open a MODFLOW 96 file locate the name file and use the ***File|Open*** command to read the file into GMS.

More about MODFLOW 96 files

MODFLOW 96 files use a name file to identify the packages files. This replaces the IUNIT array used in MODFLOW 88. The advantage of it is that the files do not need to all have the same prefix in their name. The name file is laid out as shown below. In the first column the card name is given (see MODFLOW documentation for more information). In the second colum the IUNIT number is given. This number must be unique from all other numbers. The third column gives the file name and as stated does not need to have the same prefix for every package.

Sample *.mfn file:

```
LIST   26 "run1.out"
BAS    1 "run1.bas"
BCF   11 "run1.bcf"
OC   10 "run1.oc"
DATA(BINARY)  30 "run1.hed"
DATA(BINARY)   40 "run140.ccf"
PCG   12 "run1.pcg"
RIV   15 "run1.riv"
WEL   13 "run1.wel"
RCH   20 "run1.rch"
MT3D   29 "run1.hff"
```

MODFLOW 2000, 2005[1], & MODFLOW-NWT[2]

Like the MODFLOW 96 files, MODFLOW 2000, 2005 and MODFLOW-NWT use name files rather than an IUNIT array. To know if a file is a MODFLOW 2000, 2005, or MODFLOW-NWT file look for a discretization file (*.dis). If a *.dis file exists then use the ***File|Open*** command and select the name file (*.nam or *.mfn) to read the simulation into GMS.

Sample *.mfn file:

```
# MF2K NAME file
#
# Output Files
GLOBAL 1 "easttex.glo"
LIST 2 "easttex.out"
DATA(BINARY) 30 "easttex.hed"
DATA(BINARY) 40 "easttex.ccf"
LMT6 18 "easttex.lmt"
#
# Obs-Sen-Pes Process Input Files
OBS 50 "easttex.obs"
DROB 54 "easttex.drob"
CHOB 55 "easttex.chob"
ASP 71 "easttex.asp"
#
# Global Input Files
DIS 19 "easttex.dis"
#
# Flow Process Input Files
```

```
BAS6 3 "easttex.ba6"
LPF 4 "easttex.lpf"
OC 15 "easttex.oc"
RCH 16 "easttex.rch"
WEL 9 "easttex.wel"
DRN 10 "easttex.drn"
CHD 13 "easttex.chd"
PCG 14 "easttex.pcg"
```

Changes in GMS 7.0

When GMS 7.0 or later reads a MODFLOW simulation it checks if the simulation files are in the modified GMS format. MODFLOW files created by GMS 6.5 or a later use this format. If the simulation is not in the GMS format then GMS converts it into this format.

In versions of GMS prior to 7.0, GMS would read the MODFLOW files and do the conversion. Starting with version 7.0, GMS uses a modified version of MODFLOW to read the input files and do the conversion. GMS then reads the converted files. By using MODFLOW to read MODFLOW files and do the conversion, GMS can read whatever MODFLOW can read. Conversely, if GMS cannot read it, MODFLOW probably can't either.

Conversion Steps

Depending on the version of your model, GMS will perform all or some of the following steps to convert the model into the standard GMS format.

1. **Convert MODFLOW 88 to MODFLOW 96**. If importing a MODFLOW 88 model, GMS creates a MODFLOW 96 Name file by examining the Basic package file or the GMS super file. The name file is put in the same directory where the Basic package file or super file is found. In creating the MODFLOW 96 name file, GMS assumes the unit numbers in the IUNIT array in the Basic package file are ordered according to the standard MODFLOW 88 order (as found in the MODFLOW 88 source code). GMS uses the lowest unit number not used in the IUNIT array for the List file added to the name file. If external arrays are being used, the unit number GMS uses for the List file may be the same as one used for an external array.
2. **Convert MODFLOW 96 to MODFLOW 2000**. After creating the MODFLOW 96 Name file, GMS calls mf96to2k.exe, a USGS program distributed with MODFLOW 2000 which converts MODFLOW 96 models to MODFLOW 2000. This creates some new files in the same directory as the basic package file: name_MF2k.bas, name_MF2K.bcf, and name_MF2K.nam (where "name" is the name of the MODFLOW 96 name file).
3. **Translate MODFLOW 2000 to GMS H5 Format**. GMS then calls the MODFLOW Translator to translate the simulation into GMS H5 format. This creates an H5 file in the temp directory. The user must save the GMS project in order to have a GMS H5 formatted MODFLOW simulation on disk, otherwise the temp file will be discarded.

mf96to2k

Some modifications were made to mf96to2k.exe with regards to layer elevations and confining beds so that the program could be run in a non-interactive batch mode.

Grid Elevations

When mf96to2k.exe converts a MODFLOW 88/96 simulation to a MODFLOW 2000 simulation the program creates a discretization file (DIS). This file defines the layer elevations for the model grid as well as the stress periods. In MODFLOW 88/96 a model could be defined without the need for explicitly defining the top and bottom elevations of the model grid. If the old model has grid elevations defined in the BCF file then those elevations are preserved in

the new MODFLOW 2000 DIS file. Where elevations are not defined in the old model then mf96to2k.exe would prompt the user to enter a constant elevation for the particular layer. When mf96to2k.exe is run by GMS these layer values are automatically set. After the model is read into GMS the user may need to edit these values.

Layer Confining Beds (LAYCBD)

When mf96to2k.exe converts a MODFLOW 88/96 model it also asks the user if a layer confining bed exists beneath each of the grid layers. When mf96to2k.exe is run by GMS no confining beds will be defined beneath the model layer. If the user wishes to include confining beds these can be edited in the *Global/Basic* dialog under the *MODFLOW* menu.

Files generated by other software

Other software such as Groundwater Vistas, Visual MODFLOW, and PM Win use their own file formats. However they do write out native MODFLOW files which GMS can read in. To use them make sure that the other software is saving out the files properly and then follow the steps above for the proper version of MODFLOW files.

Groundwater Vistas

To export MODFLOW files from Groundwater Vistas:

1. Open the simulation in Groundwater Vistas
    1. Select “File | Open”
    2. Navigate to and select the “*.gwv” file, then select “Open”
2. Export the native MODFLOW files from Groundwater Vistas
    1. Select “Model | MODFLOW (or MODFLOW 2000) | Create Datasets”
3. Import the name file into GMS
    1. Select “File | Open”, the “Open” macro, or just drag and drop the *.nam file in the GMS main screen.

PM Win

1. Select "Models | MODFLOW | Run"
2. Prior to MODFLOW running the model inputs will be generated.

Visual MODFLOW

Visual MODFLOW files can not be read into GMS. To use Visual MODFLOW files, you'll need to run MODFLOW from within Visual MODFLOW, and then modify the *.mfi file. See below for details.

1. Run MODFLOW from Visual MODFLOW
    1. Open the Visual MODFLOW project (vmf file if using the latest version of Visual MODFLOW) in Visual MODFLOW
    2. Select “Run” in the top menu
    3. Select “Run” again from the top menu
    4. Select “MODFLOW 2000” in the “Engines to Run” dialog, then select “Translate & Run”
    5. Select the “Close” button in the “VMEngine” window when the model is finished running
2. Modify and rename the “*.mfi” file
    1. Go to the directory where the simulation is saved on your computer
    2. Create a copy of the “*.mfi” file. Change the extension of the copy to “*.mfn”
    3. Open the *.mfn file in a text editor
    4. Comment out packages that are not supported by the USGS release of MODFLOW (for example, the “WHS” and “NDC” lines)^

5. If necessary, modify the directory that each MODFLOW file is referencing. This is necessary if the Visual MODFLOW files were not created on the computer you are on
6. Save the *.mfn file

3. Open the *.mfn file in GMS
   1. Select “File | Open”, the “Open” macro, or just drag and drop the *.mfn file in the GMS main screen
   2. The “MODFLOW Translator” will most likely appear. Select “OK” after selecting the appropriate version of MODFLOW
   3. Select “Done” when the MODFLOW Translator is finished
   4. A dialog will appear saying that a supported solver was not found in the name file and that the PCG solver has been added. This is because the solver that Visual MODFLOW uses is not compatible with the USGS version of MODFLOW, and so GMS does not use it either. Select “OK”

^Note: to comment out a package, place a pound/number sign in front of a line. See the Online Guide to MODFLOW [4] for packages that the USGS version of MODFLOW supports.

USGS MODFLOW Documentation

Here are some links to MODFLOW documentation that may be helpful.

MODFLOW 88	MODFLOW 88 (I) [8], MODFLOW 88 (II) [9]
MODFLOW 96	MODFLOW 96 (I) [10], MODFLOW 96 (II) [11]
MODFLOW 2000	MF2K Flow [2], MF2K Obs-Sen-Pes [16], HUF [13], LMG [14], LMT [15], MF2K Calibration [12]
MODFLOW 2005	MF2005 Flow Process [3]
MODFLOW-NWT	MODFLOW-NWT, A Newton Formulation for MODFLOW-2005 [4]

Notes

[1] Supported starting at GMS version 8.0

[2] Supported starting at GMS version 8.2

[3] http://www.aquaveo.com/technical-support/

[4] http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/index.html?introduction.htm

MODFLOW with HDF5

The versions of MODFLOW 2000, MODFLOW 2005[1], and SEAWAT[1] that ship with the GMS software have been modified to be able to read input data stored in HDF5 files. GMS saves some MODFLOW data to an HDF5 file that is saved with the other MODFLOW files. Some MODFLOW files will have references to the HDF5 file. For more information about HDF5, click here[2].

Advantages to HDF5

The HDF5 file format is a cross platform binary format for storing scientific data. One advantage of using HDF5 is that the data is stored in binary format so the disk reads and writes are much faster than with ASCII files (although not nearly as elegant to read). You can view the data stored in an HDF5 file by using HDFView [3] (or some other available viewer).

Another advantage of using the HDF5 libary with MODFLOW package data and array data is that HDF5 will compress the data. For example, if you have a transient simulation using the river package the typical line in a river package file would look like this:

[K] [I] [J] [STAGE] [CONDUCTANCE] [ELEVATION]

1 3 4 10.2 5.8 9.5

Then during the next stress period typically the stage would change. The line in the file would look like this:

1 3 4 10.8 5.8 9.5

So we repeated all of the data except that 10.2 changed to 10.8. With compression those repeated values do not take up much space on disk so that the resulting file is smaller.

In one example a river file that was 437 MB was saved to HDF5 format with a compression level of 1; the resulting file was 14 MB. In another example an HDF5 file that contained drain and general head data was 8 MB while the drain file was 253 MB and the general head 141 MB. Not only do the files compress extremely well but the read/write times for the HDF5 file are much faster than the ASCII files.

Changes to MODFLOW 2000 & 2005[1] code

The following subroutines in ult6.f were modified: U2DREL, U2DINT, and ULSTRD. The stream package reading routines were also modified in the str6.f file.

ult.f modifications

U2DREL and U2DINT were modified so that if the key word HDF5 was encountered when attempting to read an array then an external procedure is called to read in the data. We have added support for the following:

Explanation of variables

HDF5	a card to indicate that this is read from an HDF5 file
CNSTNT	the multiplier for the array
IPRN	print flag for the output control for MODFLOW
"FNAME"	the HDF5 file where the array is stored
"pathInFile"	path to the data set in the HDF5 file
nDim	number of dimensions that the data set has (this is 1, 2, 3)
start1	the index (NOTE: these are 0 based **not** 1) for the starting point to read the data set in the first dimension
nToRead1	the number of values to read in the first dimension
start2	the index for the starting point to read the data set in the second dimension
nToRead2	the number of values to read in the second dimension
start3	the index for the starting point to read the data set in the third dimension
nToRead3	the number of values to read in the third dimension

example: "HDF5 1.0 0 "input.h5" "Recharge/07. Property" 3 0 1 0 132 0 1"

This type of formatting will work for any HDF5 data set that has 3 dimensions or less and the data set can be a 4 byte float or an 8 byte double. The other available format that can be used with the HDF5 key word for the array reading utilities is the following:

HDF5 CONSTANT CNSTNT

example: HDF5 CONSTANT 3.0

This type of formating will assign a constant value to the array. This type of formatting may seem unnecessary. However, the constant identifier can be useful when using parameters to define arrays. Parameters will be explained in another section.

ULSTRD was also modified to read data from an HDF file. This format is specific to the types of HDF5 files that GMS creates.

GMS_HDF5_01 "FNAME" "pathInFile" SP

Explanation of variables

GMS_HDF5_01	a card to indicate that this is read from an HDF5 file
"FNAME"	the HDF5 file where the array is stored
"pathInFile"	path to the group in the HDF5 file where all of the data for the boundary condition is stored
SP	stress period number

Here is an example of a regular modflow drain file and a drain file with the HDF5 modifications.

Comparison of MODFLOW Drain files

Traditional Drain file	Drain file with HDF5
3 40 AUX IFACE AUX CONDFACT AUX CELLGRP 3 0 1 3 2 19.0 10.0 6 1.0 -1 1 4 3 19.0 10.0 4 1.0 -1 1 5 4 19.0 10.0 5 1.0 -1 3 0 1 3 2 18.9 11.0 6 1.0 -1 1 4 3 18.9 11.0 4 1.0 -1 1 5 4 18.9 11.0 5 1.0 -1 3 0 1 3 2 19.0 10.0 6 1.0 -1 1 4 3 19.0 10.0 4 1.0 -1 1 5 4 19.0 10.0 5 1.0 -1	#GMS_HDF5_01 3 40 AUX IFACE AUX CONDFACT AUX CELLGRP 3 0 0 GMS_HDF5_01 "sg_t_pest_65.h5" "Drain" 1 3 0 0 GMS_HDF5_01 "sg_t_pest_65.h5" "Drain" 2 3 0 0 GMS_HDF5_01 "sg_t_pest_65.h5" "Drain" 3

str6.f modifications

Since the STR package does not use the ULSTRD utility the str6.f file had to be modified to read the same data that ULSTRD was modified to read: **GMS_HDF5_01 "FNAME" "pathInFile" SP**.

Parameters

MODFLOW 2000 introduced the concept of parameters as native input to MODFLOW. Starting with version 6.5, GMS no longer writes out native MODFLOW parameters (except when clusters are defined) and the use of the MODFLOW PES process is not available from within GMS. Even when native MODFLOW files are exported from GMS, native MODFLOW parameters are not used (except when clusters are defined) and instead the parameter starting values are written. However, GMS still supports PEST and users may create parameters in the GMS interface as they have been able to do previously. Parameters are created in GMS by assigning a "key" value (usually a negative number) to a MODFLOW input. When MODFLOW is running and calls our external routine to read in the HDF5 a check is made in the data that is read from the HDF5 file. If one of the parameter "key" values is found in the data then the parameter value is substituted into the array or list.

By adopting this approach it was much easier to support transient parameters and very large sets of pilot points.

Also, adopting this approach allows GMS users to use parameters with the BCF package. This feature is not available with the MODFLOW PES process.

Pilot Points

In previous versions of GMS, pilot points were supported by using the multiplier arrays in MODFLOW. Beginning with version 6.5 the pilot point interpolation takes place with in our external routine that is called by MODFLOW. For example, if MODFLOW calls our routine to read an HK array and that array has parameter *key* values that are associated with a parameter that is defined using pilot points then our routine will perform the pilot point interpolation and substitute the appropriate value. This includes any log interpolation that the user has specified.

Reading MODFLOW files which include HDF5 data

When GMS writes out the MODFLOW files for the list based packages, the first item written to the file is #GMS_HDF5_01. When GMS reads these MODFLOW files with this special comment, it does not read any more of the package file and the data from the *.h5 file will be used.

When GMS saves the RCH or EVT package with parameter that are defined with cluster (and instances). Then a different special comment is written to the top of the file: #GMS_PARAM_CLUSTERS. If GMS is reading a project file that includes a MODFLOW simulation then when this special comment is encountered GMS will not read any more of the package file. However, if a user is reading a MODFLOW model (not a project file) then the rest of this package file will be read and new data sets will be created on the 3D grid that are used to define the clusters used by the parameters.

Exporting Native MODFLOW Files

To export native MODFLOW ASCII files from GMS 6.5 (or later), use the following steps:

1. Open a project in GMS (6.5 or later).
2. In the 3D Grid Module, select ***MODFLOW | Export Native MF2K text...*** (GMS 8.3 and below) or ***MODFLOW | Advanced | Export Native MF2K text...*** (GMS 9.0 and above).
3. In the window that appears, double-click the Name file of the MODFLOW model that you want to convert to ASCII format.
4. A DOS prompt will appear. Press the Enter key when the executable is finished.
5. A folder called **Out_Mf2k** is created in the same folder as the name file you selected. **Out_Mf2k** contains all the MODFLOW input files in ASCII format.

If the DOS prompt does not appear after selecting the name file, then go to Edit|Preferences... and select Models. Verify that the **Gms2Mf2k** executable (the application that converts MODFLOW files from HDF5 to ASCII format) has the correct path next to it. If it doesn't, select ***Browse...*** and locate the executable. It will probably be located at **C:\Program Files\GMS 8.1\models\mf2k\Gms2Mf2k.exe**.

Notes

[1] Supported starting at GMS version 8.0

[2] http://hdf.ncsa.uiuc.edu/HDF5/

[3] http://hdf.ncsa.uiuc.edu/hdf-java-html/hdfview/index.html

Unsupported MODFLOW Features

MODFLOW Versions

The supported MODFLOW versions include:

- MODFLOW 2005 (Supported starting at GMS version 8.0. Read/Write)
- MODFLOW 2000 (Read/Write)
- MODFLOW 96 (Read and convert to MODFLOW 2000. No write)
- MODFLOW 88 (Read and convert to MODFLOW 2000. No write)

The unsupported MODFLOW versions include:

- MF2K-GWM
- MF2K-VSF
- MF2K-FMP

Processes

For GMS 6.5 and 7.0 the following processes are not supported:

- PES (This process is not needed since GMS uses PEST for parameter estimation)
- SEN (This process is not needed since GMS uses PEST for parameter estimation)

Packages

- See Packages Supported in GMS. All other packages are unsupported (but we are always working on adding support for more packages). For any package not currently supported in GMS, the file associated with that package will be ignored when the model is imported. However, GMS keeps track of unsupported packages it encounters when reading the name file and, when the project is saved, GMS lists the unsupported packages in the name file and copies the unsupported package files from the old directory to the new directory.

Options

The following MODFLOW options are not supported:

- XSECTION
  - GMS does not support models that use the XSECTION option on line 1 of the BA6 file.
- Quasi-3D confining bed (GMS 6.5.x and before)
- File formats: GMS 6.5.x (and earlier versions) can read most regularly formatted files but MODFLOW supports more formatting options than GMS does. Beginning with version 7.0, MODFLOW is used to import non-GMS MODFLOW simulations (thus, all MODFLOW formats can be imported).

Parameters

MODFLOW 2000 introduced the concept of parameters as native input to MODFLOW. Starting with version 6.5, GMS no longer writes out native MODFLOW parameters (except when clusters are defined) and the use of the MODFLOW PES process is not available from within GMS. Even when native MODFLOW files are exported from GMS, native MODFLOW parameters are not used (except when clusters are defined) and instead the parameter starting values are written. However, GMS still supports PEST and users may create parameters in the GMS interface as they have been able to do previously. Parameters are created in GMS by assigning a "key" value (usually a negative number) to a MODFLOW input. When MODFLOW is running and calls our external routine to read in

the HDF5 a check is made in the data that is read from the HDF5 file. If one of the parameter "key" values is found in the data then the parameter value is substituted into the array or list.

By adopting this approach it was much easier to support transient parameters and very large sets of pilot points.

Also, adopting this approach allows GMS users to use parameters with the BCF package. This feature is not available with the MODFLOW PES process. Other unsupported parameter options:

- HFB, SFR (GMS 7.0.x and before)
- STR, CHD (GMS 6.5.x and before)
- Multiple clusters for array based parameters (GMS 6.5.x and before)
- Parameter Instances (GMS 6.5.x and before)

Interpolate to MODFLOW Layers

In this dialog the user can select various 2D scatter point data sets and associate them with MODFLOW input data. GMS will then interpolate from the 2D scatter point data to the MODFLOW input data. This is often useful to define the layer elevations of a MODFLOW model. Click here for more information on MODFLOW layer elevations.

The user associates 2D scatter point data with MODFLOW data by selecting a data set in the list on the left of the dialog and selecting an item from the MODFLOW data list on the right and then selecting the **Map** button. The association between the data sets and the MODFLOW data is shown in the spread sheet labeled *Data set => MODFLOW data*.

The *MODFLOW data* group box contains options to allow the user to pick which MODFLOW data they would like to interpolate to. *Elevations* refers to the top and bottom elevations of the 3D grid. *Heads* refers to the starting heads. *Flow package data* refers to the various input arrays for the LPF or BCF packages (HK, VK...). *Recharge* refers to the recharge rate specified in the RCH package. *CHD BCs* refers to the starting and ending heads associated with existing CHD boundary conditions in the MODFLOW model.

The **Automap** button will try to automatically map the data sets to the MODFLOW data by matching names and layer numbers. The Unmap button is used unmap the selected item(s) in the spread sheet. The **Unmap All** button is self explanatory.

The Interpolation Options button will bring up the *2D Interpolation Options* dialog.

Transient Interpolation

If a 2D scatter point data set is transient and the user is interpolating to MODFLOW data that does not vary with time then the user will select a time step from that data set to interpolate to the MODFLOW data. When the user has selected a time step the **Apply Selected Time To All Transient Data Sets** button will undim. This button allows the user to set the selected time of all of the transient data sets to be the same as the currently selected time.

If the current MODFLOW model is transient and the user is interpolating to Recharge then interpolation will occur for each stress period defined in the MODFLOW model. For a particular stress period, the closest data set time step whose time is less than the beginning of the stress period is used. Figure 1 illustrates this process.

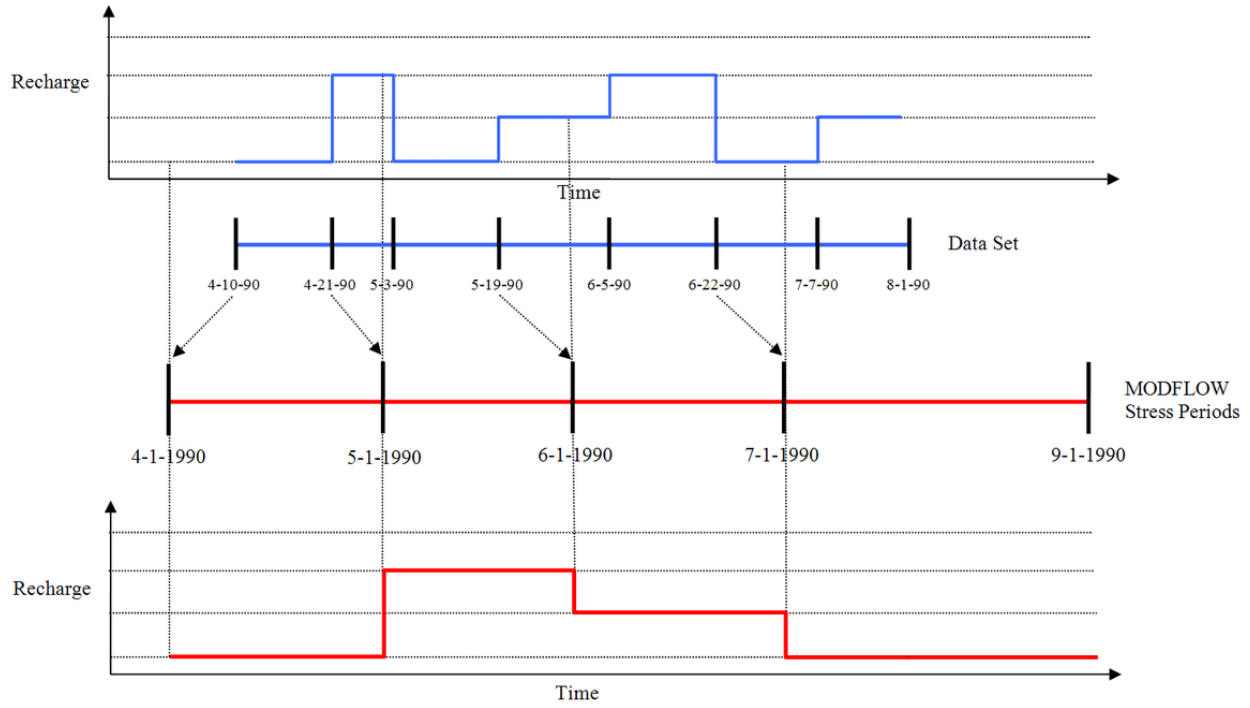


Figure 1: Transient interpolation of Recharge

If the current MODFLOW model is transient and the user is interpolating to CHD BCs then interpolation will occur at the beginning and the end of each stress period (because a start head and an end head are specified for each CHD BC). If there is no data set time step that matches the beginning or the end of the stress period then GMS will linearly interpolate between data set time steps. Figure 2 illustrates this process.

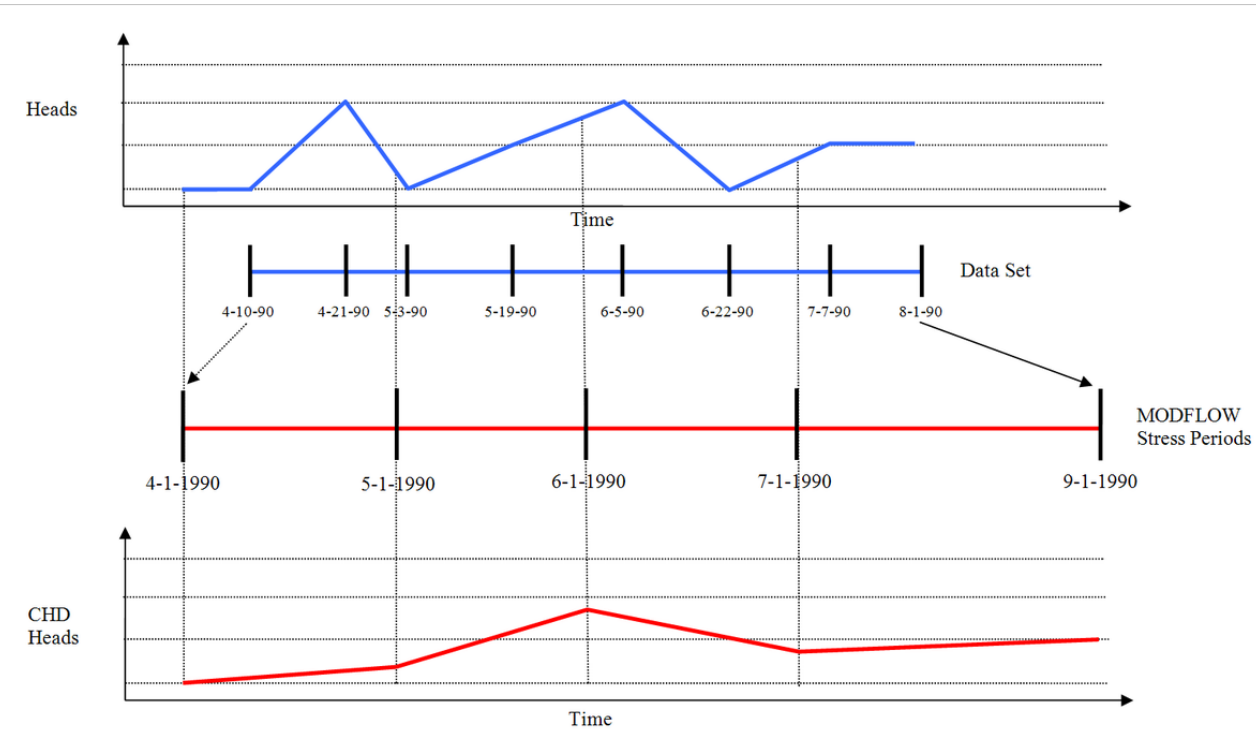


Figure 2: Transient interpolation of CHD BCs

If the current MODFLOW model is transient and the user is interpolating to GHB BCs then interpolation will occur at the beginning of each stress period. If there is no data set time step that matches the beginning or the end of the

stress period then GMS will linearly interpolate between data set time steps. Figure 3 illustrates this process.

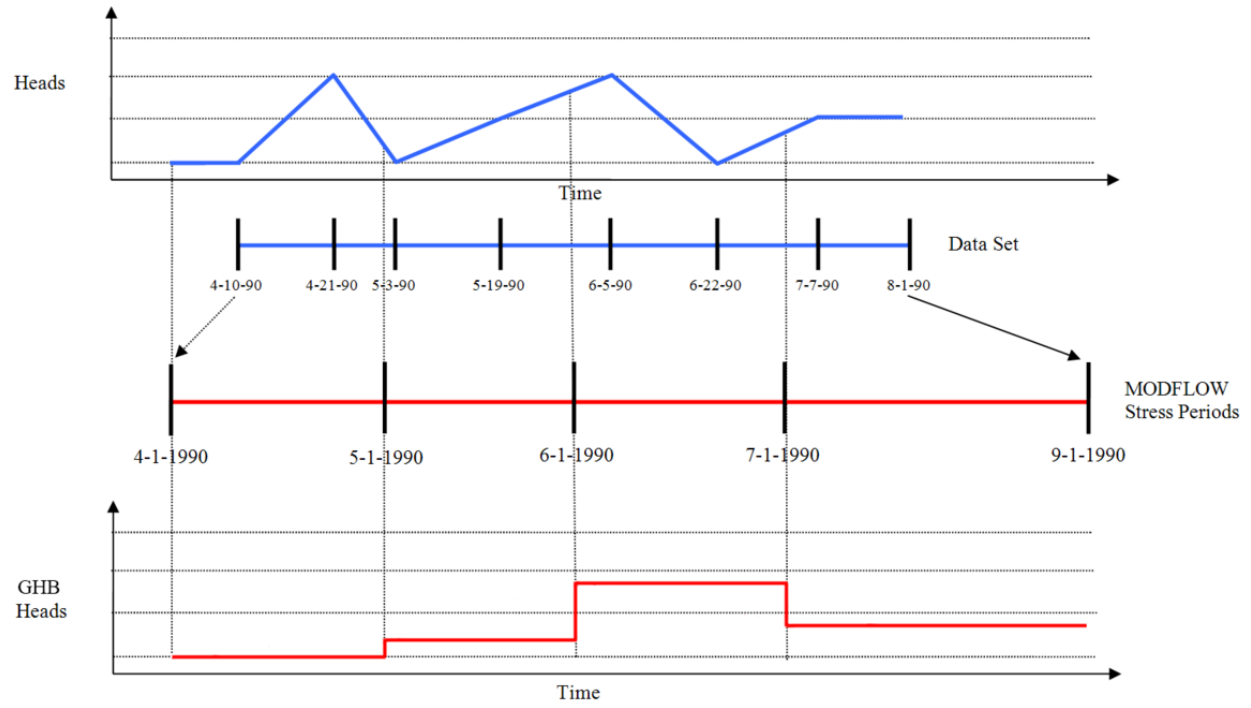


Figure 2: Transient interpolation of GHB BCs

MODFLOW Layers to 2D scatter points

This dialog allows the user to create a scatter point set and data sets of the current MODFLOW simulation.

The user can limit the number of scatter points created by turning on the **Only create scatter points within selected coverage option** and selecting the appropriate coverage. This is often used when converting between a regional model and a local scale model.

Layer Subdivision

The layers of the current MODFLOW simulation can be subdivided by specifying the *Number of local model layers* for each layer in the current 3D grid.

The user can select which MODFLOW data sets to create by turning off/on the toggles below the *Create data sets of* text. Data sets for layer elevations, flow package data (HK, HANI, VK, SY, SS...), Recharge, and Heads can be created. The user must select a 3D grid data set in order to create a data set for the Heads (most often this will be the MODFLOW solution from the regional model).

The Recharge and Head data sets can be transient if the regional model was transient. The user can also select a Start and End time to limit the number of time steps for these data sets.

Bias Layer 1

An option to bias the thickness of the new layer 1 is also available. This can be useful if equally subdividing layer 1 of the regional model would result in cells where the elevation would be above the computed heads. Thus, the user can choose to bias the thickness of the new layer 1 to ensure that the top layer in the new model will not be dry.

MODFLOW Source/Sink Dialog

The Sources/Sinks dialog allows the user to edit both point sources/sinks and areal sources/sinks.

Point Sources/Sinks

The MODFLOW stresses can be categorized as point sources/sinks and areal sources/sinks. The point sources/sinks include rivers, wells, drains, and general head. Point sources/sinks are not assigned using arrays. Rather, they are associated with individual cells. Two methods are used to define point source/sink data. The simplest method is to define them as part of a MODFLOW conceptual model defined in the Map module. Another method is to assign them by selecting a set of cells and using the Sources/Sinks command.

The Sources/Sinks command is used to both assign and edit river, drain, general head, and well type sources/sinks. Before selecting the Cell Sources/Sinks command, a set of cells should be selected using the cell selection tools. Once the command is selected, the Point Sources/Sinks dialog appears.

Creating New Sources/Sinks

A new instance of a source/sink of a particular type is created by selecting the Add button for the type. This creates a new source/sink and displays a default value or set of values for the source/sink in the edit fields on the right side of the dialog. If the simulation is steady state, normal edit fields are used to enter the values. If the simulation is transient, buttons appear which can be used to bring up the XY Series Editor. A value is entered for each of the defined stress periods.

Multiple instances of a source/sink can be created by repeatedly selecting the Add button. Each cell can contain multiple sources/sinks of a particular type or a mixture of several types.

Editing Sources/Sinks

An existing source/sink can be edited by selecting the name of the source/sink in the source/sink list. The values associated with the highlighted source/sink are displayed in the spread sheet.

Deleting Sources/Sinks

An instance of a source/sink may be deleted by selecting the source sink from the list and selecting the Delete button.

Constant Values

Several of the parameters shown in the Point Sources/Sinks dialog, such as elevation and conductance, are not likely to change during a transient simulation. A constant value can be entered for these parameters in the XY Series Editor and the resulting curve is a flat line.

Areal Sources/Sinks

The Areal Sources/Sinks command is used to edit recharge and evapotranspiration parameters on a cell-by-cell basis. Before selecting the Areal Sources/Sinks command, a set of cells should be selected using the cell selection tools. Recharge and evapotranspiration parameters are applied to vertical columns rather than to individual cells. Therefore, to edit the value for a vertical column, any cell in the column can be selected. Once the Areal Sources/Sinks command is selected, the Areal Sources/Sinks dialog appears. The options in the dialog are as follows:

Packages

If the Recharge package has not been activated (using the Packages dialog which is accessed through the Global Options\Basic Package dialog) the Recharge portion of the Areal Sources/Sinks dialog is dimmed. Likewise, if the Evapotranspiration package has not been activated, the Evapotranspiration portion of the dialog is dimmed.

Editing Values

The edit fields to the right of each option are used to enter the values of the parameters associated with each type. The fields are standard edit fields if the simulation is steady state and are graphic windows displaying a time series if the simulation is transient. Clicking on the window brings up the XY Series Editor. The XY Series Editor is a general purpose editor for entering curves or lists of pairs of data (e.g., rainfall rate vs. time). Once a curve is defined in the editor, it is displayed graphically in the window.

Layers

The Layer option in the Recharge portion of the dialog is only active (undimmed) if the Recharge at Specified Vertical Cells option is chosen in the Recharge Package dialog. Likewise, the Layer option in the Evapotranspiration portion of the dialog is only active if the ET at Specified Vertical Cells option is chosen in the Evapotranspiration Package dialog.

Editing Multiple Cells

After a set of source/sink parameters has been defined, it is often necessary to change one of the parameters of a subset of the cells (vertical columns).

For example, suppose the Evapotranspiration package has been activated and each vertical column was assigned a unique value of elevation, extinction depth, and maximum evapotranspiration rate. Suppose that it becomes necessary to change the extinction depth of a large subset of the vertical columns to a constant value while leaving the other parameters unchanged. The Areal Sources/Sinks dialog has been designed so that it can be used to change one of the parameters without altering the other parameters.

If more than one cell is selected when the Areal Sources/Sinks dialog is brought up, the available edit fields appear with a checkerboard pattern if the values in the cells are not all identical. Before editing a parameter, click on the field to switch it from multi-select mode to normal mode. When the OK button is selected after the parameters have been edited, only the parameters that have been selected are changed. For example, in the case of changing the extinction depth, if the extinction depth is edited, the extinction depth of all of the vertical columns associated with the selected cells is changed to the new value but the individual values of elevation and maximum evapotranspiration rate are left unchanged.

6.3.3. MODFLOW Post-Processing

MODFLOW Display Options

The properties of all MODFLOW data that GMS displays on the screen can be controlled through the MODFLOW tab of the Display Options dialog. This dialog is opened by right clicking on the MODFLOW entry in the Project Explorer and selecting the Display Options command. It can also be accessed from the from the Display menu, the MODFLOW menu, or the Display Options macro. The following table describes the display options available for the 3D Grid module.

Display Option	Description
Wells, Drains, Rivers, Streams, General head, Constant head, Transient head	These items on the left side of the dialog represent source/sink objects. If the check box just to the left of each source/sink name is selected, a symbol is displayed at the center of each cell with that type of source/sink. The symbol for each source/sink is displayed to the left of the check box. The symbol can be changed by selecting the symbol button. This brings up the symbol editor dialog. The symbol editor contains a list of available symbols. The dialog can also be used to edit the size and color of the symbol.
Horiz. flow barriers	The Horiz. flow barrier option displays a line at the location of each horizontal barrier. The attributes (thickness, color, etc.) can be edited by clicking on the small window to the left of the Horiz. flow barrier toggle.
Dry cells	If the Dry cells option is selected, the chosen symbol will be displayed at the location of all dry cells in the grid. A MODFLOW solution must be imported to GMS prior to displaying dry cells. When a cell goes dry during a MODFLOW simulation, the HDRY value defined in the BCF Package is assigned as the head value for the cell. If an HDRY value is encountered in the active scalar data set when the display is refreshed, the cell is assumed to be dry.
Water table	If the Water table option is selected, the water table defined by a MODFLOW solution is superimposed on the layer geometry when a grid cross section is displayed in orthogonal mode. The water table is defined as the head value in the uppermost active cell. If the water table display is on, all contours (head, concentration, etc.) are clipped so that they lie at or below the water table. This option is only available if the True Layer mode is active.
Mark flooded cells	The Mark flooded cells option is used in conjunction with the True Layer approach to defining layer data. With the True Layer approach, the top elevation is entered for each layer, regardless of the layer type. With many models, the top layer is an unconfined layer and the top elevation represents the ground surface. For unconfined layers, the top elevation array is not read by MODFLOW. Only the bottom elevation array is used in the calculations. MODFLOW assumes that the top layer extends to an infinite height. It is often the case that the computed water table elevation exceeds the elevation of the ground surface. The Mark flooded cells option is used to draw a symbol at the center of all cells where the computed water table elevation is greater than the top elevation of the top layer in the grid.
Lake cells	If the Lake cells option is selected, a symbol is draw in the center of each cell representing a lake. The symbol, the symbol size, and symbol color can be adjusted by clicking on the button to the left of the Lake cells toggle.
Lake ID's	If the Lake ID's option is selected, each cell representing a lake will display the lake ID in the center of the cell. The font, font size, and font color can be adjusted by clicking on the button to the left of the Lake ID's toggle.
Display symbol legend	If the Symbol legend option is selected, a legend showing each of the symbols associated with sources/sinks, dry cells, and flooded cells is displayed in the lower right corner of the GMS window.
Display hydrogeologic units	The Display hydrogeologic units option is used to display HUF data. This option only works if the current display mode is Ortho Mode. This mode can be turned on in the Display menu.
Check All	By clicking this button, all of the display options are turned on.
Check None	By clicking this button, all of the display options are turned off.

MODFLOW Post Processing Viewing Options

In addition to generating and editing the MODFLOW input files, GMS can also be used for post-processing the solution files computed by MODFLOW. The solution files computed by MODFLOW include head, drawdown, and CCF files. By default, the head and CCF files are automatically generated. The output options are controlled in the MODFLOW *Output Control* dialog.

No-Flow and Dry Cells

When a MODFLOW simulation is solved, MODFLOW writes out a head or drawdown value for every cell of the finite difference grid to the solution files. However, some of the cells are either outside the problem domain or they have gone dry during the course of the simulation. These cells are flagged by MODFLOW in the output file by writing special values for the cells. The value assigned to inactive cells is the No flow head value specified in the *Global Options/Basic Package* dialog. The value assigned to cells which have gone dry is the Head assigned to dry cells value defined in the BCF, LPF or HUF package dialogs. If the MODFLOW data are in memory when the solution is read in, GMS will automatically use the No flow head and Head assigned to dry cells values to define active/inactive cells for post-processing.

Layer Contours

In most cases, the best way to display computed head and drawdown is with layer contours. Layer contours are generated by selecting the Layer Contours option in the 3D Grid Display Options dialog. This option is automatically turned on whenever a MODFLOW solution is read into GMS. The **Mini-Grid Toolbar**, which is part of the Tool Palettes, can be used to switch between layers.

Viewing Computed Fluxes

The CCF file that is part of the MODFLOW solution contains useful information about the computed flux rates between the aquifer and external sources and sinks. A special set of tools are provided for viewing computed fluxes.

Summation of Fluxes on Arcs and Polygons

GMS writes the necessary files so that MODFLOW will output the computed flow for boundary conditions created in the Map module. These computed flows can be viewed by selecting the appropriate feature object (river arc, etc) and then looking at the Status Bar. For an object with an assigned observed flow, the observed flow value and the residual error are displayed in addition to the computed flow. For objects without an observed flow, only the computed flow is shown.

This cannot be done for SFR stream arcs since the SFR package does not participate in the Observation Process.

Calibration Targets and Statistics

For objects with an observed flow, a Calibration Target can be plotted on the object. The calibration target provides a graphical representation of the calibration error. Calibration targets are described in section 14.5. The display of flow calibration targets is turned on by selecting the Display Options command in the Feature Objects menu when the Local Source/sink coverage is the active coverage.

Flow Budget for Selected Cells

If a MODFLOW model is built without using the conceptual model approach (directly from the grid), the computed fluxes corresponding to a user-defined set of cells can still be displayed. This is accomplished by selecting a set of cells and selecting the ***Flow Budget*** command from the *Data* menu in the 3D Grid module. This command brings up the *Flow Budget* dialog. This dialog lists the complete flow budget for the selected cells.

GMS also includes a **Zone Budget** tool to view the computed flows into (out of) user defined zones.

Vector Plots

If a CCF file has been imported as described above, a vector plot can be generated to illustrate the flow field computed by MODFLOW. The CCF file contains flows through each of the cell walls in the grid, i.e., the flow from each cell to each of its six surrounding cells.

Vectors are generated by right-clicking on the CCF file in the Project Explorer and selecting the ***CCF->Velocity Vectors*** command. The cell top and bottom elevations as well as the porosity are used when calculating the velocity vectors. Therefore, for GMS to compute the vectors, a MODFLOW simulation must exist in GMS. Although porosity is not an input to a MODFLOW model, the porosity can be specified per cell, using the cell properties dialog, whenever a MODFLOW simulation exists.

The vectors are computed by reading the CCF file to get the net flow through each grid cell face. Each component of the velocity vector is computed by dividing the flow through the cell face by the saturated area of the face multiplied by the porosity. For example, the I, J, K direction components of the vector are calculated as follows:

- $$vector_i = \frac{flow_i}{(saturated_{Area_i})(porosity)}$$
- $$vector_j = \frac{flow_j}{(saturated_{Area_j})(porosity)}$$
- $$vector_k = \frac{flow_k}{(area_k)(porosity)}$$

The saturated area may be less than the area of the cell face if the computed head is below the top elevation of the grid cell. The velocity vector is set to 0.0 in cells that are inactive, dry (the computed head is below the cell bottom elevation), or have inappropriate elevations (the top elevation is below the bottom elevation).

Prior to version 8.2.

To generate a vector data set from the CCF file, right click on the CCF data set in the Data Tree and select the **Generate vectors** option from the pop up menu. A flow vector is generated at each cell center by computing a vector sum of the flows through the six walls of the cell. The resulting vectors can be plotted by selecting the Vectors option in the *3D Grid Display* Options dialog.

Viewing the Printed Output File

Two types of output are produced by MODFLOW: a printed output file and a set of solution files (head, drawdown, CCF). Before reading in the solution files, it is often useful to examine the printed output file. In some cases, MODFLOW may crash or not complete its run successfully. You can usually determine if the run was completed successfully by viewing the printed output file. When viewing the file you should check to make sure that a solution was output for all stress periods and time steps you are expecting. In some cases MODFLOW will also output to the listing file a description of any problems which may have occurred.

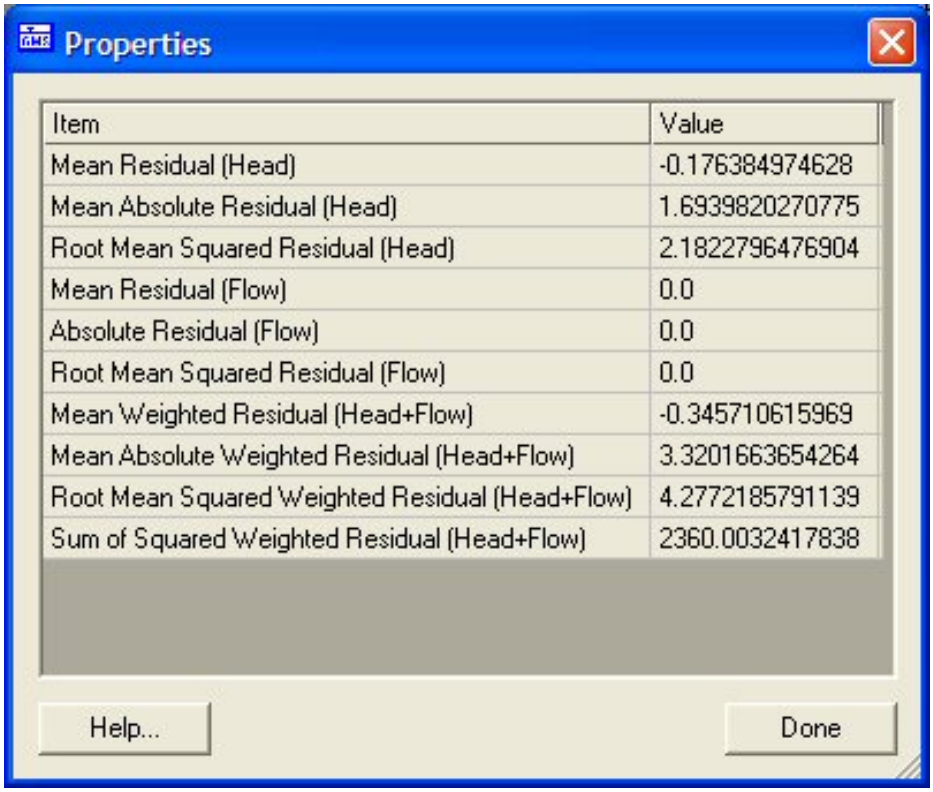
GMS provides two ways to view the text files produced by MODFLOW and the other analysis codes:

1. When a solution is read into GMS, the text output files are placed into the data tree. Double clicking on their file icons in the Project Explorer will bring up the text files in a text editor.
2. Any text file can be viewed by selecting the ***Edit File*** command in the *File* menu. A File Browser appears and the selected file is opened in a text editor.

MODFLOW Solution Properties Dialog

The MODFLOW Properties Dialog Box is opened by right clicking on the MODFLOW solution folder in the project explorer.

The data in this dialog come from the *._os, *._ww, *._r, *._w files computed by the MODFLOW Observation process. The computation from MODFLOW will include any observed flows combined with the observed heads to calculate a single error value. In a transient model, the error value includes all of the observations at the various times. The error shown in this dialog is different from the error found in the Error Summary Plot.



Comment on different error values

- Mean Residual - Average error for the observations. This can be misleading because the positive and negative errors can cancel.
- Mean Absolute Residual - Mean of the absolute error values for the observations. This is a true mean, not allowing positive and negative errors to cancel.
- Root Mean Squared Residual - RMS is calculated by taking the sum of the square of the errors for the observations and then taking its square root. This tends to give more weight to cases where a few extreme error values exist.
- Sum of Squared Weighted Residual - This is the error value that is minimized by a PEST run.

Point head observation errors

Mean Residual (Head).

Mean Absolute Residual (Head).

Root Mean Squared Residual (Head).

Flow observation errors

Mean Residual (Flow).

Mean Absolute Residual (Flow).

Root Mean Squared Residual (Flow).

Combined head and flow error values

Mean Weighted Residual (Head+Flow).

Mean Absolute Weighted Residual (Head+Flow).

Root Mean Squared Weighted Residual (Head+Flow).

Sum of Squared Weighted Residual (Head+Flow).

Saving and Reading a MODFLOW Simulation

Saving a MODFLOW Simulation

Once a MODFLOW simulation has been created and checked for potential problems with the Model Checker, the next step is to save the simulation to disk and run MODFLOW. MODFLOW simulations are saved using the ***Save*** and ***Save As*** commands in the *File* menu.

Selecting the ***Save*** command saves the GMS project including the model simulation. By default the model simulation will be saved to the same location as the GMS project. However, in the Save dialog the path for the model simulation can be specified.

A MODFLOW simulation is actually saved to a set of input files. The MODFLOW super file is used to store extra data used by GMS but not used by MODFLOW. The super file also contains the path to the name file. The names of all of the input and output files associated with a simulation are saved in the name file. When MODFLOW is launched, the name of the super file is automatically passed to the MODFLOW executable.

When a MODFLOW simulation is saved, the names of the other MODFLOW input files are automatically patterned after the name of the super file. For example, if the super file is named sampmod.mfs, the other files are named sampmod.bas, sampmod.bcf, etc.

The user can adjust the output options in the *Output Control* dialog

The version of MODFLOW 2000 that ships with the GMS software has been modified to be able to read and write input data stored in HDF5 files. For more information see MODFLOW with HDF5.

Reading a MODFLOW Simulation

Once a MODFLOW simulation has been saved by GMS using the ***Save*** command in *File* menu, the entire simulation can be read back into GMS using the ***Open*** command in the *File* menu.

MODFLOW simulations can be read in individually (*.mfs) or as part of a project (*.gpr). They can also be imported by using the MODFLOW name file. The extension for the name file must be changed to *.mfn.

Reading a Completed MODFLOW Solution

When you are using the Model Wrapper to control your MODFLOW run, you can use the **Read MODFLOW solution** toggle at the bottom of the dialog to automatically read in the corresponding solution.

You can also read in solution files generated by MODFLOW using the ***Read Solution*** command in the *MODFLOW* menu. This command brings up the a file browser and prompts you to choose a MODFLOW super file (pre GMS 7.0) or a MODFLOW name file (GMS 7.0+).

Cell Properties

The *cell properties* dialog allows the user to edit cell properties. Most cell properties are associated with a model such as MODFLOW or MT3D. If no models exist in the GMS project them the *cell properties* dialog will only allow editing of the material assigned to the grid cell.

MODFLOW

Several input arrays defining parameters such as starting head, IBOUND, hydraulic conductivity, and transmissivity are defined in the Global/Basic and BCF, LPF, or HUF packages. These arrays can be edited in the Basic and BCF/LPF/HUF Package dialogs, or they can be initialized using a conceptual model in the Map module. In many cases however, it is necessary to view or edit the values on a cell-by-cell basis. This can be accomplished using the ***Cell Properties*** command in the *MODFLOW* menu.

Before selecting the ***Cell Properties*** command, a set of cells should be selected using the cell selection tools. Once the command is selected, the *MODFLOW Cell Attributes* dialog appears.

The parameters for the selected cells are changed by typing in new values in the edit fields. If more than one cell is selected when the ***Cell Properties*** command is selected, the available edit fields will be left blank (unless all values are the same for that parameter). To edit one of the parameters, click on the edit field to be edited. When the **OK** button is selected, only the parameters whose edit fields that have data are changed. This makes it possible to change one of the parameters (e.g., transmissivity) for all of the selected cells while leaving the other parameters unchanged.

NOTE: When you are using materials to define the MODFLOW model, the Cell Properties dialog will show the material properties relating to the material of the selected cell. You will not be able to edit these values on a cell-by-cell basis, but you can either edit the material type for this cell if the active material set is the default material set, or you can change the material properties for the material (which affects every cell that uses that material).

MT3DMS/RT3D/SEAM3D

MT3D inputs that vary on a cell by cell basis can also be editing using this dialog and editing the data in the MT3D tab.

MODFLOW World File

A MODFLOW world file is a plain text file containing the geographic location of a MODFLOW model. The world file contains 3 lines including the origin, rotation about the z axis, and the path of a projection file. The world file is found in the same directory as the name file. The MODFLOW world and projection files are automatically written by GMS when the project has a global projection.

Format

```
ORIG x y z
ROTZ theta
PRJ_FILE "file_path"
```

The ORIG line contains the space separated x, y, and z coordinates of the outside corner of the model cell at the first column and last row.

The ROTZ line contains the counter-clockwise (looking down) rotation of the model about the origin coordinate in degrees.

The PRJ_FILE line contains the absolute or relative path to the model's projection file which ends in with a *.prj extension. The file path is sourounded by double quotes.

Sample

```
ORIG 612086.0 3429376.55 230.0
ROTZ 90.0
PRJ_FILE "modfmap.prj"
```

Error Summary Plot

An Error Summary plot is one of the plot types that can be created by the Plot Wizard. See the Error Summary plot section on the Plot Wizard page for a basic description. The Error Summary plot is used to display a text listing of the mean error, mean absolute error, and root mean squared error for an observation measurement in a coverage. The error values may be listed for a single time step of a data set or for all time steps.

Error types

Mean Error: This is the average error for the points. This value can be misleading since positive and negative errors can cancel.

Mean Absolute Average: This is the mean of the absolute values of the errors. It is a true mean, not allowing positive and negative errors to cancel.

Root Mean Square: This takes the sum of the square of the errors and then takes its square root. This norm tends to give more weight to cases where a few extreme error values exist.

Time matching

When the measurement is transient (i.e., observed heads at various times) then it is very unlikely that the output times from the model match the times when the field measurements were taken. In this case GMS will interpolate an observed value at the model output time. If the model output time is before the first field measurement for a particular point then the interpolated value is the first measurement. Similarly if the model output time is after the last field measurement then the interpolated value is the last measurement. When the model output time is between the first and last measurement then GMS will find the 2 closest field measurments to the model output time and use linear interpolation to compute the "observed" value at that time.

MODFLOW errors

The Error Summary Plot is most useful with models that do not make error computations from observation data. MODFLOW does compute error computations from observation data, and these errors are available in the MODFLOW properties dialog. Therefore, when using MODFLOW, you should use the MODFLOW properties dialog and not the Error Summary Plot. The errors shown in the Error Summary Plot are not the same as those found in the MODFLOW properties dialog due to the time matching and interpolation issues described above. The MODFLOW properties dialog shows the errors computed by MODFLOW for the observations at the actual observation times and is therefore superior. The errors reported by MODFLOW have nothing to do with the model output times, only observation times.

Plot creation

Error Summary plots are created in the Plot Wizard by setting the plot type to Error Summary. A sample plot is shown in the figure.

Error Summary Plot Options

After the plot type is set in the first step of the Plot Wizard, the Next button is clicked to move to the second step of the Plot Wizard.

Coverage: Displays the name of the coverage where the current data for the plot is coming from.

Measurement: This is the name of the current measurement, created in the Feature Objects | Attributes dialog, being plotted.

Feature Objects: Displays which feature object is utilized in the current plot, points or arcs.

Zone Budget

In previous versions of GMS, it has been possible to view a detailed MODFLOW flow budget for a set of selected cells using the Flow Budget command in the Data menu. Now, the flow budget can be summarized based on user-defined zones. This provides a capability quite similar to the USGS ZoneBudget tool. However, the calculations are all done inside GMS using the CCF file generated by MODFLOW.

Defining Zones

The first step in using this utility is to identify the model zones by assigning a zone budget id to each of the cells in the grid. The zone budget id is an integer value. It can be associated with polygons in a MODFLOW conceptual model in the map module. The zone budget id property is listed in the Areal Properties column of the Coverage Setup dialog. These IDs are then assigned to the appropriate grid cells when the ***Map->MODFLOW*** command is selected. The IDs can also be assigned directly to cells by selecting a set of cells and selecting the Cell Properties command in the MODFLOW menu.

A Zone Budget IDs item is also included just below the MODFLOW icon in the Project Explorer window. Clicking on this icon displays the zone budget IDs and double-clicking brings up the zone budget id array in the spreadsheet editor.

Viewing the Flow Budget

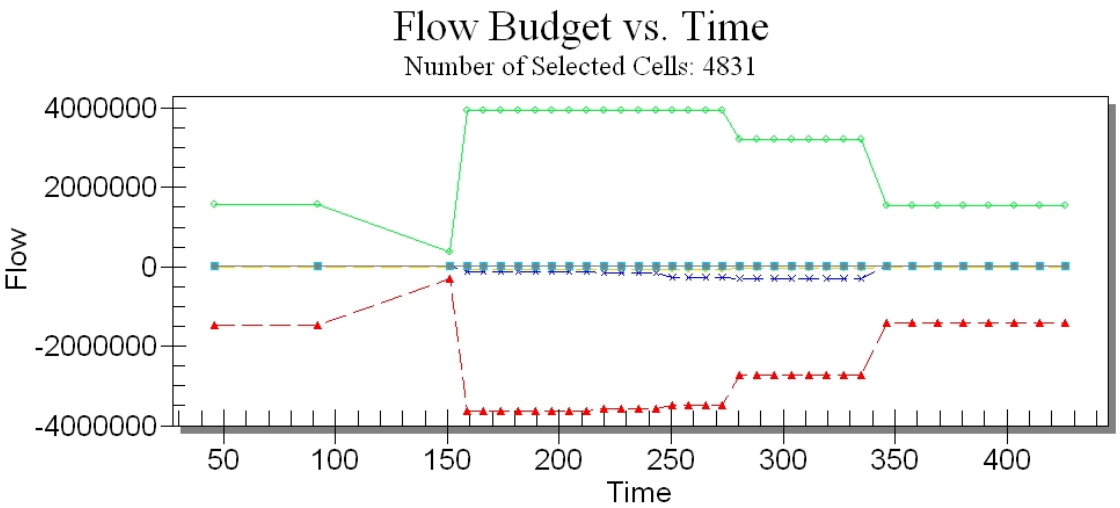
Once the zone budget IDs have been assigned, the flow budget for each zone can be viewed by selecting the Flow Budget command in the MODFLOW menu. This brings up the Flow Budget dialog. There is a new zone selector combo box at the top of the dialog. The flow budget associated with the selected zone is shown in the table. The combo box includes an "All zones" option that displays a summary for all zones in the model. Also, turning on the **Use all timesteps toggle** will create a flow budget report for each time step in the current MODFLOW solution.

Zone 1 Use all

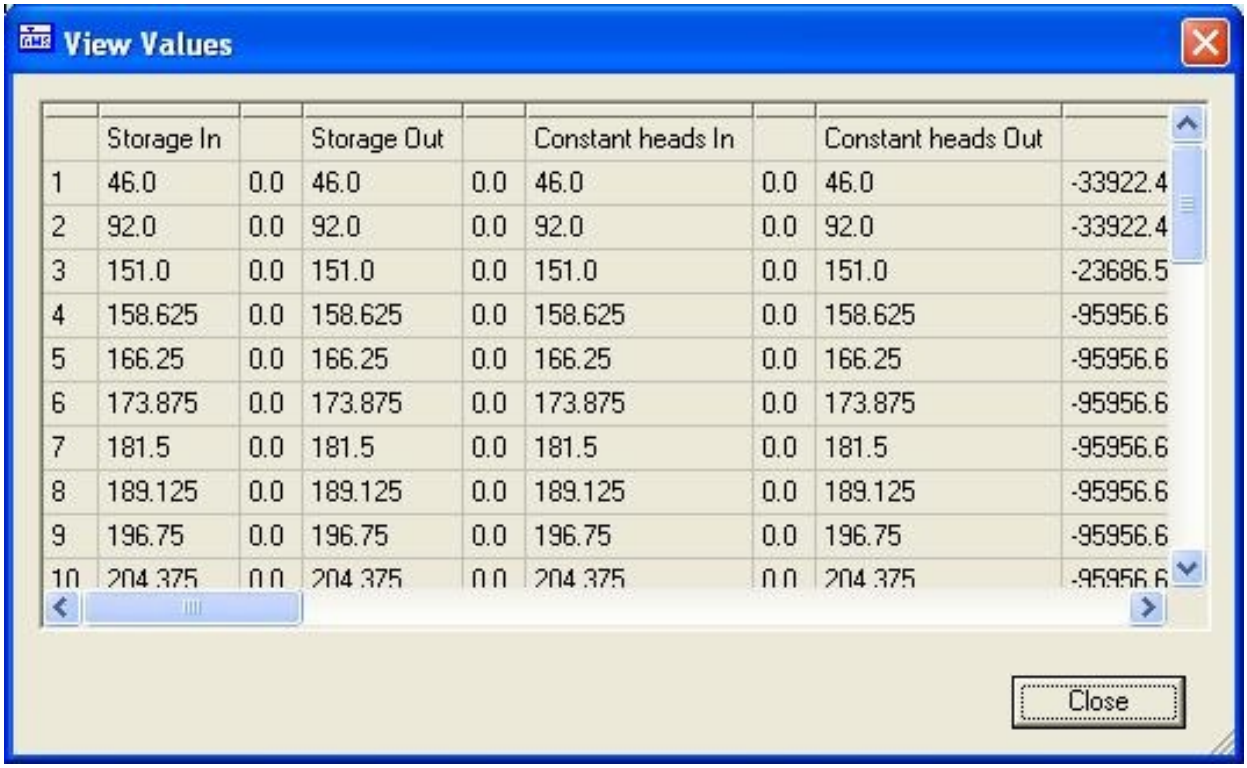
Budget Term	Flow (ft^3/d)
Flow Budget for Zone 1	
IN:	
Constant heads	0.0
Rivers	0.0
Wells	0.0
Recharge	137744.224617
Zone 2 to zone 1	13754.908902884
Zone 3 to zone 1	1155.7250471115
Total IN	152654.858567
OUT:	
Constant heads	4686.9240722656
Rivers	133345.99891376
Wells	1000.0
Recharge	0.0
Zone 1 to zone 2	3849.4356174469
Zone 1 to zone 3	9772.7417325974
Total OUT	152655.10033607
SUMMARY:	
IN - OUT	-0.241769075394

Viewing in a Plot File

For a transient model you may use the flow budget vs. time plot to view the flow budget for any number of cells.



By right clicking on the plot and select the view values option, GMS will generate a table of the flow budget for the different time steps.

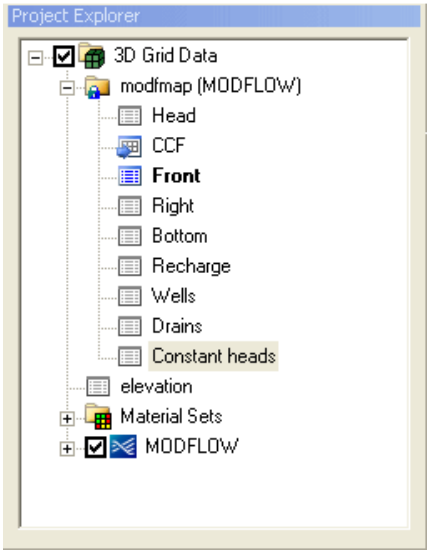


	Storage In		Storage Out		Constant heads In		Constant heads Out	
1	46.0	0.0	46.0	0.0	46.0	0.0	46.0	-33922.4
2	92.0	0.0	92.0	0.0	92.0	0.0	92.0	-33922.4
3	151.0	0.0	151.0	0.0	151.0	0.0	151.0	-23686.5
4	158.625	0.0	158.625	0.0	158.625	0.0	158.625	-95956.6
5	166.25	0.0	166.25	0.0	166.25	0.0	166.25	-95956.6
6	173.875	0.0	173.875	0.0	173.875	0.0	173.875	-95956.6
7	181.5	0.0	181.5	0.0	181.5	0.0	181.5	-95956.6
8	189.125	0.0	189.125	0.0	189.125	0.0	189.125	-95956.6
9	196.75	0.0	196.75	0.0	196.75	0.0	196.75	-95956.6
10	204.375	0.0	204.375	0.0	204.375	0.0	204.375	-95956.6

Viewing the MODFLOW CCF File

There are two new options to view MODFLOW cell-to-cell flow (CCF) file output:

1. The CCF file can be viewed in a spreadsheet by right-clicking on the CCF file in the Project Explorer and selecting the View Values command.
2. The CCF file can also be converted to a set of data sets. One data set would be created for drains (if they exist), one for rivers etc., and 3 for cell-to-cell flow (flow right, flow back, flow down).



CCF data sets displayed in the Project Explorer

ZONEBUDGET

ZONEBUDGET	
Model Info	
Model type	Analysis of MODFLOW cell to cell flow files
Developer	USGS, [1]
Documentation	ZONEBUDGET 1.0 [2] ZONEBUDGET 3.01 [3]
Tutorials	MODFLOW Tutorials

ZONEBUDGET is USGS program that reads cell to cell flow data produced by MODFLOW and calculates water budgets for subregions of the modeled area. GMS has an interface to ZONEBUDGET available from the ***MODFLOW | Flow Budget*** menu command. This command brings up the Flow Budget dialog and one of the available tabs in the dialog is USGS ZONEBUDGET. GMS supports version 3.01 of ZONEBUDGET.

When the user brings up the ZONEBUDGET tab they will be analyzing the CCF file from the active MODFLOW solution. All ZONEBUDGET inputs and outputs will be written to the same location as the CCF file.

GMS has its own internal tools for analyzing CCF data. These tools are explained here.

ZONEBUDGET OPTIONS

- **Title** - This is a title that is printed to the listing output file.
- **Output**
  - **Listing File** - This specifies that ZONEBUDGET will produce a listing file as output. This was the only kind of output that the first version of ZONEBUDGET produced.
  - **Multiple Outputs** - Version 3 of ZONEBUDGET has the option to produce multiple output files.
    - **ZBLST** - ZONEBUDGET will create a listing file as part of its output.
    - **CSV** - ZONEBUDGET will create a comma separate value (CSV) file as part of its output. For each time for which a budget is requested there is one line for each input term and each output 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.
    - **CSV2** - ZONEBUDGET will create another CSV file as part of its output. 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.
  - **Output times**
    - **all** - Every time step in the MODFLOW CCF file will be processed.
    - **specified** - With this option selected the user can select individual time steps from the CCF file for ZONEBUDGET to process. When the user clicks on the **Times** button a spread sheet comes up that allows the user to select the time steps.
- **Composite Zones** - ZONEBUDGET allows users to combine zones into "Composite Zones" and then information about the composite zone is printed to the listing file.
  - **Number of zones** - This specifies the number of composite zones.
  - **Edit Zones** - This button brings up a dialog where the user can create composite zones. A composite zone is defined by a name that is 10 characters or less in length and a list of the zone ids separated by a comma. For

example, when analyzing a model with zones 1, 2, 3, and 4, composites zone could be defined as follows:

Name	Zone IDs
zone_top	1, 2
zone_bot	3, 4

- **Run ZONEBUDGET** - This launches ZONEBUDGET with the specified input options.
- **View** - This allows the user to load ZONEBUDGET outputs. The options available include LST, ZBLST, CSV, and CSV2. The contents of the output file are loaded into a text window or a spread sheet in the space below the View check box.
- **Open Containing Folder** - This button brings up Windows Explorer opened to the directory with the ZONEBUDGET output.

References

[1] http://water.usgs.gov/nrp/gwsoftware/zonebud3/zonebudget3.html
[2] http://gmsdocs.aquaveo.com/ofr90392.pdf
[3] http://gmsdocs.aquaveo.com/zonbud3.pdf

Viewing Computed Fluxes

Once a set of observed flows has been entered, the next step is to run the MODFLOW model, read in the solution, and compare the computed flows to the observed flows. The computed flows are part of the MODFLOW output.

Summation of Fluxes on Arcs and Polygons

GMS writes the necessary files so that MODFLOW will output the computed flow for boundary conditions created in the Map module. These computed flows can be viewed by selecting the appropriate feature object (river arc, etc) and then looking at the Status Bar. For an object with an assigned observed flow, the observed flow value and the residual error are displayed in addition to the computed flow. For objects without an observed flow, only the computed flow is shown.

Calibration Targets and Statistics

For objects with an observed flow, a calibration target can be plotted on the object. The calibration target provides a graphical representation of the calibration error. Calibration targets are described in section 14.5. The display of flow calibration targets is turned on by selecting the ***Display Options*** command in the *Feature Objects* menu when the Local Source/sink coverage is the active coverage.

Flow Budget for Selected Cells

If a MODFLOW model is built without using the conceptual model approach (directly from the grid), the computed fluxes corresponding to a user-defined set of cells can still be displayed. This is accomplished by selecting a set of cells and selecting the ***Flow Budget*** command from the *Data* menu in the 3D Grid module. This command brings up the *Flow Budget* dialog. This dialog lists the complete flow budget for the selected cells.

6.4. MODPATH

MODPATH

MODPATH	
Model Info	
Model type	particle tracking
Developer	USGS, [1]
Documentation	MODPATH Manual [1]
Tutorials	MODPATH Tutorials

MODPATH is a particle tracking code that is used in conjunction with MODFLOW. After running a MODFLOW simulation, the user can designate the location of a set of particles. The particles are then tracked through time assuming they are transported by advection using the flow field computed by MODFLOW. Particles can be tracked either forward in time or backward in time. Particle tracking analyses are particularly useful for delineating capture zones or areas of influence for wells.

A complete description of MODPATH is beyond the scope of this help file, however, because of the user-friendly interface in GMS, an intimate knowledge of MODPATH is not required to effectively do particle tracking in GMS. For a more complete knowledge of MODPATH, refer to the MODPATH documentation (Pollock, 1994).

MODPATH was developed by the U.S. Geological Survey. Version 5.0 of MODPATH is supported in GMS. The version of MODPATH distributed with GMS is the original public domain version distributed by the USGS, with minor modifications to accommodate GMS.

MODPATH Links

- MODPATH Particle Tracking
- MODPATH Particle Sets
- MODPATH Zone Codes
- MODPATH Display Options
- Exporting Pathlines

References

[1] http://gmsdocs.aquaveo.com/mpathref.pdf

MODPATH Particle Tracking

Requirements

Before you can do particle tracking with MODPATH, you must have:

1. A MODFLOW simulation in memory.
2. A MODFLOW solution in memory computed using MODFLOW 2000 with a valid head and flow field.

If the Conceptual Model approach is used to build the MODFLOW model, the same conceptual model can be used to initialize some of the input data for MODPATH. Both the zone codes and porosities can be defined using polygons in a MODFLOW / MT3D / MODPATH Layer Attributes type coverage. The values are assigned to the cells when the ***Map -> MODPATH*** command is selected.

Steps

Once you have a MODFLOW solution, all that is necessary to do particle tracking is to:

1. Create particle starting locations.

As soon as you create the particle starting locations GMS immediately does a number of things depending on the *Run MODPATH automatically for steady state models* option in the *MODPATH General Options* dialog. If the option is on and the MODFLOW model is steady state.

Automatic option on

1. GMS saves the MODPATH input files.
2. GMS launches MODPATH and passes it the input files.
3. GMS waits for MODPATH to compute the pathlines.
4. GMS then reads in and displays the pathlines.

All this is done automatically and behind the scenes and usually takes just a second or two. Thus, pathlines will appear almost immediately after you define the particle starting locations. If MODPATH encountered problems attempting to generate the path lines, the errors will be displayed in the MODPATH Errors dialog.

Automatic option off

If the *Run MODPATH automatically for steady state models* option is off, or the MODFLOW model is transient, you must save and run MODPATH manually after creating particle starting locations before pathlines will appear. This is to prevent having GMS spend lots of time updating pathlines because MODPATH can take a considerable amount of time with large, transient models. The *MODPATH|Run MODPATH* menu command or equivalent toolbar macro can be used to run MODPATH.

Generating Particles

There are two ways to generate particle starting locations in GMS, both available via the MODPATH menu:

Generate Particles at Wells - Accessed in the *MODPATH* menu. This command automatically generates particle starting locations in cells containing wells. The specified number of particle starting locations are distributed evenly in a horizontal circle around the center of the cells containing the wells. You specify the number of starting locations per cell, and whether you want starting locations created in extraction well cells, or injection well cells.

Injection Wells - If this option is selected, particles are created in cells with wells that have a positive flow rate. The tracking direction for the current particle set is changed to forward.

Extraction Wells - If this option is selected, particles are created in cells with wells that have a negative flow rate. The tracking direction for the current particle set is changed to backward.

Selected Wells - This option makes it possible to generate particles at either all wells or only at wells within selected cells.

Generate Particles at Selected Cells - Accessed in the *MODPATH* menu. This command opens the *Generate Particles* dialog, and when you select **OK**, particles are created in all the selected cells according to the options specified.

Number of Particles - If the **More options** toggle is not selected, you can use the slider to change the number of particles created per cell. The minimum is 1, and the maximum depends on the option being used to distribute the particles. The number of particles jumps as the slider is moved in order to create an even distribution of particles. If the **More options** toggle is selected, the slider is not available, and the user has more control over the total number of particles and how they are distributed.

Distribute Particles - There are three options for distributing the particles within the selected cells.

- **Within Cell** - With this option, the particles are distributed in the interior of the cells.
- **On Cell Faces** - With this option, the particles are distributed on the faces of the cells.
- **Distribute Starting Points on Water Table Surface** - With this option, the particles are restricted to the top face only. When using this option, you should be sure to select the cells corresponding to the location of the water table surface.
- **More Options** - The More options toggle expands the dialog, allowing you to further define how particles are distributed within the selected cells.

(These commands are only available if a MODFLOW CCF solution generated by MODFLOW 2000 exists, and you have 3D grid cells selected.)

Transient MODFLOW Solution

For each time step, particle paths are computed just as for the steady state case until the end of the time step is reached. A new velocity distribution is then calculated for the next time step and the computation of particle paths is resumed. The computation of paths forward or backward, boundary conditions, and the path line termination criteria are handled the same as for steady state flow.

MODPATH Particle Sets

MODPATH particles are grouped into sets. For each set, you can specify the name of the set, the tracking direction, the tracking duration, and if the particles in the set should be displayed.

Grouping particles into sets increases the power and flexibility of particle tracking. For example, several particle sets, some tracking backward and some forward can all be displayed at once. Or, several particle sets, each with different tracking times, can all be displayed at the same time. This can be used to show nested capture zones.

Active Particle Set

One particle set is always designated as the active particle set, and there is never more than one active particle set. Whenever particles are created, they are added to the active particle set. Particles can only be deleted from the active particle set - to delete particles in a particle set that is not active, you must first make it active.

Order

The order that particle sets are listed in the *Data Tree* corresponds to the order they are displayed. Thus, particle sets that are listed at the top are displayed on top of particle sets listed further down. The order can be changed by dragging the particle sets.

Creation / Deletion

If a particle set is deleted, all the particles in the set are deleted.

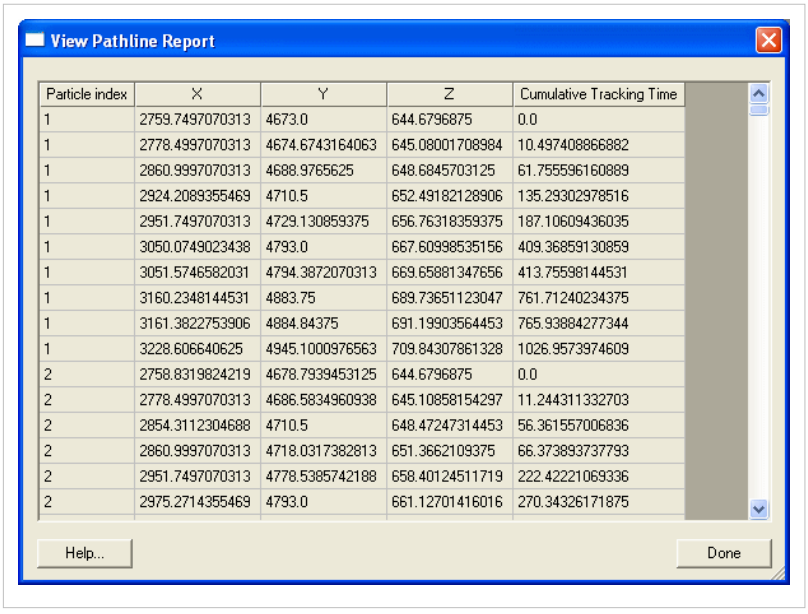
If there are no particle sets, and you create particles, a particle set is automatically created.

Pathline Export

See Exporting Pathlines.

Spreadsheet Report

In addition to the text file export, we have an option for generating a tabular report directly within GMS. This report is accessed by right clicking on a particle set in the Project Explorer and selecting the ***View Pathline Report*** command. This command brings up the following dialog:



MODPATH Zone Codes

When post-processing the results of the MODPATH simulation, the colors of the paths or particles can be varied depending on the zone code of the cell in which the particle started or in which the particle terminated. Zone codes are assigned using the IBOUND array in the MODFLOW interface. In other words, unique values of the IBOUND array (100, 200, 300, etc.) are assigned to the cells of the grid to define the zone codes. The zone code array can be edited by clicking on the ***Zone Code Array*** command in the *MODPATH* menu. This command is only available if a MODFLOW simulation exists.

Cell Properties

The Zone Code for each cell can also be edited by selecting a cell and then choosing the ***Cell Properties*** command from the *MODPATH* menu. In addition to the zone code, cell porosity can be edited in the *Cell Properties* dialog.

MODPATH Display Options

A set of display options unique to the MODPATH input data and MODPATH solutions is provided in GMS. These options are accessed through the ***Display Options*** command in the *MODPATH* menu. This command is only available if a MODFLOW simulation exists. This command brings up the Particles tab of the *3D Grid Display Options* dialog. The following table describes the display options available for the MODPATH model.

Display Option	Description
Starting locations	The starting locations for the particles can be turned on and off. The symbol style, color and size can also be adjusted.
Starting location indices	The starting locations indices for the particles can be turned on and off. The font style, color and size can also be adjusted.
Ending locations	The ending locations for the particles can be turned on and off. The symbol style, color and size can also be adjusted.
Pathlines	The pathlines can be toggled on and off, and the pathline style and color can be adjusted. The pathline color can be set to the default color, or the color corresponding to the starting, ending, or cell zone codes of the pathlines. The "Cell zone code" option causes the pathline to change color as it passes through cells with different zone codes.
Direction arrows	Direction arrows can be displayed along the pathlines. The size of the arrow heads can be set by specifying the Length in pixels. The arrows are displayed along the pathline at an interval corresponding to the Length specified.
Zone codes	Colors can be associated with zone codes. If the Auto compute colors option is selected, GMS will automatically pick colors to go with each unique zone code. Otherwise, you can specify the color you want to associate with each zone code. These colors are used if the Pathline Color option is set to Starting zone code or Ending zone code.

Capture zones	GMS groups pathlines together into capture zones. A polygon representing the outer boundary of the pathlines is found and can be outlined, or filled. The following options are available relating to the capture zones: • **Delineate by well** With this option, all the pathlines originating from a cell containing a well will be grouped together into one capture zone. All wells with the same name are included in the same capture zone. • **Delineate by zone code** With this option, all pathlines originating from the same zone code are grouped together into capture zones. This option could be used to create a single capture zone for several wells that have different names. The cells containing the wells would need to be assigned the same zone code. This option could also be used to find the "capture zone" for a zone of cells where the cells all have the same zone code. • **Thin triangle ratio** GMS triangulates the pathlines in a capture zone to determine the capture zone boundary. Depending on the length and shape of the pathlines, it may be necessary to adjust the Thin triangle ratio to get a good looking capture zone. Increasing the value causes more area around the edges to be included. Decreasing the value causes less area around the edges to be included.

Exporting Pathlines

MODPATH pathlines can be exported from GMS in a few different ways:

Capture Zones -> Arcs

The *MODPATH | Capture Zones -> Arcs* command will convert the capture zone outline to feature arcs, creating a separate coverage for each well. Coverages can be exported as a shapefile or converted to CAD data. Capture zones are defined using the "Delineate by well" and "Delineate by zone code" options in the MODPATH Display Options dialog.

Pathlines -> Arcs

The *MODPATH | Pathlines -> Arcs* command works similar to the *MODPATH | Capture Zones -> Arcs* but instead of converting the capture zone boundary, all of the pathlines in the capture zone are converted.

Starting Locations -> 3D Scatter Points

Starting locations can be converted to 3D scatter points and vice versa. If the *MODPATH | Starting Locations -> 3D Scatter Points* menu command is selected, a new 3D scatter point set will be created from each particle set that is visible. If the command is executed by right-clicking on a particle set in the Project Explorer, a new 3D scatter point set will be created from only that particle set.

Tab delimited file

Pathlines can be exported by right-clicking on a particle set in the Project Explorer and selecting the *Export* option. This saves the pathline geometry to a tab-delimited text file that can be imported directly into Excel:

Spreadsheet report

You can bring up a spreadsheet report showing the pathline XYZ data in GMS. See MODPATH Particle Sets, Spreadsheet Report.

MODPATH Commands

Menu Command	Description
Display Options...	
Generate Particles at Wells...	
Generate Particles at Selected Cells...	
Cell Properties...	
Porosity...	
Porosity Confining Beds...	
Zone Code Array...	
General Options...	
Capture Zone → Arcs	
Recompute Pathlines	

6.5. MT3DMS

MT3DMS

MT3DMS	
Model Info	
Model type	3D Transport Model
Developer	-
Documentation	MT3DMS Manual [1] MT3DMS v5.3 Supplemental User's Guide [2]
Tutorials	MT3DMS Tutorials

MT3DMS is a modular three-dimensional transport model for the simulation of advection, dispersion, and chemical reactions of dissolved constituents in groundwater systems (Zheng, 1990). MT3DMS uses a modular structure similar to the structure utilized by MODFLOW. MT3DMS is used in conjunction with MODFLOW in a two step flow and transport simulation. Heads and cell-by-cell flux terms are computed by MODFLOW during the flow simulation and are written to a specially formatted file. This file is then read by MT3DMS and utilized as the flow field for the transport portion of the simulation.

MT3DMS is a newer version of the MT3D model distributed with earlier versions of GMS. MT3DMS differs from MT3D in that it allows for multi-species transport, supports additional solvers, and allows for cell-by-cell input of all model parameters.

A complete description of MT3DMS is beyond the scope of this reference manual. It is assumed that the reader has a basic knowledge of MT3DMS and has read the MT3DMS documentation (Zheng, 1990). Only the details of the GMS graphical interface to MT3DMS are described herein.

GMS supports MT3DMS as a pre- and post-processor. The input data for MT3DMS is generated by GMS and saved to a set of files. These files are then read by MT3DMS when MT3DMS is executed. MT3DMS can be launched from the GMS menu. The output from MT3DMS is then imported to GMS for post-processing.

A special version of MT3DMS is distributed with GMS. This version of MT3DMS has been modified to output GMS data set files.

The RT3D, SEAM3D and PHT3D models are special versions of MT3DMS that have been customized to simulate reactive transport problems. The interfaces to MT3DMS, RT3D, SEAM3D and PHT3D are all contained in the *MT3D* menu.

MT3DMS Links

- MT3D Packages
- Building an MT3DMS Simulation
- Saving an MT3DMS Simulation
- Importing an MT3D Simulation

References

[1] http://gmsdocs.aquaveo.com/mt3dms.pdf
[2] http://gmsdocs.aquaveo.com/mt3dms_v5_supplemental.pdf

MT3D Packages

MT3DMS is divided into a series of components called "packages." Each package performs a specific task. Some of the packages are always required for a simulation, and some are optional. The input for each package is contained in a separate text file. The MT3DMS packages supported in the GMS interface are listed in the following table:

Package Name	Abrev Name	Decription	Always Req'd?
Basic Transport Package	BTN	Handles basic tasks that are required by the entire transport model. Among these tasks are definition of the problem, specification of the boundary and initial conditions, determination of the step size, preparation of mass balance information, and printout of the simulation results.	YES
Advection	ADV	Solves the concentration change due to advection with one of the three mixed Eulerian-Langrangian schemes included in the package: MOC, MMOC, or HMOC	NO
Dispersion	DSP	Solves the concentration change due to dispersion with the explicit finite difference method.	NO
Sink & Source Mixing	SSM	Solves the concentration change due to fluid sink/source mixing with the explicit finite difference method. Sink/source terms may include wells, drains, rivers, recharge, and evapotranspiration. The constant-head boundary and general-head-dependent boundary are also handled as sink/source terms in the transport model.	NO
Chemical Reactions	RCT	Solves the concentration change due to chemical reactions. Currently, the chemical reactions include linear or nonlinear sorption isotherms and first-order irreversible rate reactions (radioactive decay or biodegradation).	NO
Generalized Conjugate Gradient Solver	GCG	This package can be used to implicitly solve the dispersion, source/sink, and reaction terms of the transport equation.	NO
Transport Observation	TOB	Outputs concentration at observation points and mass fluxes at groups of source/sink boundary conditions.	NO
PHT3D-PHREEQC Interface	PHC	Used by PHT3D to define options for species related to PHREEQC geochemical reactions.	NO

MT3D Source/Sink Mixing Package

The *Source/Sink Mixing Package* dialog is used to assign concentrations to point sources/sinks (wells, river/streams, specified head, general head) and areal sources/sinks (recharge, evapotranspiration). In most cases, the concentration is assigned to the incoming water when the sources/sinks are acting in the source mode, i.e., contributing water to the system. In sink mode, the concentration of the outgoing water is equal to the concentration of groundwater in the aquifer and the concentrations assigned to the sources/sinks have no effect. The only exception is evapotranspiration. Even though evapotranspiration always acts in sink mode, a concentration can be specified. Generally, the assigned concentration is zero which only allows pure water to leave the aquifer.

Source/Sink Mixing Package dialog

Maximum number of Sources/Sinks in Flow Model

MT3DMS needs to know the maximum number of sources/sinks in the flow model. This number is simply the total number of cells in the MODFLOW model that have a source or sink defined at them. This number is computed automatically.

Point sources/sinks spreadsheet

Values for the concentration as well as the type of source or sink and the location of each of the point source/sink cells are displayed and edited in the spreadsheet. Since the concentration data are time dependent, one value is defined for the concentration at each stress period. Concentration values are displayed in the spreadsheet for the current stress period only. The current stress period is displayed above the spreadsheet and can be changed. If the concentration values for a previous stress period are the same as those used for the current stress period, the **Use previous** option may be used. When the **Use previous** option is selected, the fields in the spreadsheet cannot be edited.

A column is provided for each of the species concentrations. Changing the source/sink type for one stress period at a cell will automatically change the type for the remainder of the stress periods at the same cell.

Point sources/sinks can be added and removed from the list by selecting the **Add** and **Delete** buttons. However, when adding new point source/sink, it is usually more convenient to select the 3D grid cells and use the ***MT3D\|Point Sources/Sinks*** menu command.

Initializing Point Source Sinks from MODFLOW

An option is included in the *Source/Sink Mixing Package* dialog to initialize the point sources/sinks to be used in the MT3DMS simulation directly from data that have already been defined in a MODFLOW simulation. If a MODFLOW simulation is currently in memory, the buttons in the *Initialize point sources/sinks from MODFLOW* dialog can be used. Each button is labeled with a different source/sink type, corresponding to the MODFLOW point sources or sinks. Selecting one of the buttons automatically adds to the list of point sources/sinks. For example, if the Well button is selected, GMS creates a new well source/sink for each cell where a well is defined in the MODFLOW simulation currently in memory. The initial concentration of each of the new well sources/sinks is zero. In order to utilize the source/sink initialization buttons, the following conditions must be met:

1. The MODFLOW package corresponding to the source/sink type to be initialized must have been selected in the MODFLOW Packages dialog.
2. Point sources or sinks of the type to be initialized must have been defined in MODFLOW.

Specified Concentration Boundary Conditions

When entering the concentrations for a specified concentration cell, it is sometimes necessary to specify the concentrations of some of the species but allow the concentrations for the remaining species to vary. This can be accomplished by specifying a negative concentration for the species that are to vary.

Areal Sources/Sinks

Recharge and evapotranspiration are known as areally distributed sources and sinks. This is because a value for concentration must be entered for each species for every vertical column of cells in the finite difference grid. This essentially means that a two dimensional array of concentration values must be defined for each species for both recharge and evapotranspiration, depending upon which options are utilized. The buttons labeled Recharge and Evapotranspiration bring up the Areal Source/Sink Array dialog.

Reset

The Reset button deletes all of the data currently defined in the *Source/Sink Mixing package* and restores the package parameters to the default values.

Conceptual Model Input

In some cases, the simplest way to define both point and areal sources/sinks is with an MT3DMS conceptual model in the Map module. Concentrations can be assigned directly to points, arcs, and polygons; points representing point sources/sinks and polygons representing recharge and evapotranspiration zones. These concentrations are copied directly to the appropriate cells/arrays in the *Source/Sink Mixing package* when the conceptual model is converted to the numerical model with the ***Feature Objects | Map -> MT3DMS*** command.

Basic Transport Package Dialog

The first step in setting up an MT3DMS simulation is to define the data for the Basic Transport package. The information defined in the Basic Transport package includes the computational time intervals (stress periods), an array defining which cells are inactive and which cells have constant concentration, an array defining aquifer porosity, and array of starting concentration values. The input data for the Basic Transport package must be entered before editing any of the other packages in the MT3DMS simulation. The *Basic Transport Package* dialog contains the following options:

Headings

A brief description of the model can be entered in the two lines provided at the top of the Basic Transport Package dialog. This information is printed to the ASCII listing file output by MT3DMS.

Model Selection

The Model section in the middle of the *Basic Transport Package* dialog is used to select which transport model is to be used. The menu commands and packages and options that are available depend on which model is selected. All MT3D-based transport models are contained in the *MT3D* menu. See the RT3D, SEAM3D and PHT3D pages for more information on those transport models.

Stress Periods

As is the case with MODFLOW, the computational time intervals for an MT3DMS simulation are called "stress periods". Concentrations at boundary conditions or source/sink terms can only change at the beginning of each stress period. Stress periods are subdivided into time steps and time steps are subdivided into transport steps. The **Stress Periods** button on the left of the *Basic Transport Package* dialog is used to bring up the *Stress Period* dialog. If a transient MODFLOW simulation is used, the stress periods and time steps used for MT3DMS are initialized to coincide exactly with those defined for MODFLOW. If a steady state MODFLOW simulation is used, any set of stress periods may be utilized for MT3DMS.

The *Stress Periods* dialog is identical to the *MODFLOW Stress Periods* dialog except for two fields. In addition to the stress period definition required by MODFLOW, MT3DMS also requires a transport step size and a maximum number of transport steps allowed for one time step. These values are defined for each stress period. If a value of zero is entered for the transport step size (the default), MT3DMS will automatically calculate an appropriate transport step size. Furthermore, if the value for the transport step size entered by the user is larger than the value computed by MT3DMS, the MT3DMS value will be used. The transport step size times the Max transport steps must be longer than the total simulation length.

Output Control

Options for printing and saving the results from an MT3DMS simulation are also included in the Basic Transport package. The MT3DMS output control options are modified by selecting the Output Control button on the left side of the *Basic Transport Package* dialog. This brings up the *MT3D Output Control* dialog.

One of the output options is an unformatted (binary) concentration file which is used for post-processing by GMS. This option is selected using the toggle at the bottom of the dialog. With the version of MT3DMS included with GMS, the concentration file is saved directly from MT3DMS as a GMS binary scalar data set file.

Another option is to Print or save at specified times. When this option is selected, the Times button is undimmed. Selecting the **Times** button brings up a spreadsheet that enables users to specify the times that the output will be printed or saved. The spreadsheet can be quickly initialized by selecting the **Initialize Values** button at the bottom of the dialog. This button brings up the *Initialize Time Steps* dialog. This dialog is composed of edit fields that will automatically populate the times that MT3D data will be saved or printed.

Packages

The **Packages** button on the left of the Basic Transport Package dialog brings up the *Packages* dialog. This dialog is used to specify which of the packages are to be used in the simulation. The check box to the left of the package name is selected to signify that a package will be utilized as part of the simulation. Some of the packages are used by RT3D or SEAM3D and are dimmed for MT3DMS simulations.

Define Species

MT3DMS is a multi-species transport model. It can track the migration and concentration of several species at once. The **Define Species** button is used to define the number of species in the simulation and the name and type of each species. The button brings up the *Define Species* dialog.

The species are listed in the box on the left side of the dialog. Species are added and deleted using the **New** and **Delete** buttons. The name of a selected species can be edited. The **Mobile** toggle is used for RT3D and is dimmed for MT3DMS simulations.

The species names are not used by the MT3DMS code. They are only used in GMS to simplify the model input. In MT3DMS, all species are identified by an integer ID. The species names are saved to the MT3DMS super file (*.mts). When building a new simulation, it is sometimes useful to use the same set of names used in a previous

simulation. This can be accomplished by selecting the Import button and selecting the MT3DMS super file used by the previous simulation. This automatically loads in the species names to the list.

Units

All MT3DMS input parameters must be entered using a consistent set of units. The Units button brings up a dialog which can be used to specify a standard unit for length, time, mass, force, and concentration. The selected units are used by GMS to post the appropriate unit labels next to each of the input fields in the MT3DMS interface. These labels serve as a reminder to the user of the correct units. The units must be consistent with the units used in the MODFLOW simulation.

CINACT

The CINACT value is written to the MT3DMS solution file wherever an inactive concentration cell exists (ICBUND=0). This value should be selected so that it will not likely be a valid concentration computed from MT3DMS. The default value of -999 is generally sufficient.

Use Materials for Porosity and Long. Dispersivity

If this option is selected, the porosities and longitudinal dispersivities specified in the Materials dialog will be used in the MT3DMS model.

HTOP Equals Top of Layer 1

In some cases it is useful to explicitly define the HTOP array separately from the top elevation array for layer 1 defined in the Global Options package. If the toggle entitled HTOP equals top of layer 1 is turned off, an HTOP array can be explicitly defined. This option should be used if the top of layer 1 is substantially higher than the computed water table. In such cases, using the top of layer 1 could lead to significant error (see MT3DMS Reference Manual).

Another option would be to use the default approach and lower the value of the layer 1 top elevation array. For unconfined layers, this array is not used by MODFLOW anyway. The only reason to keep the HTOP array separate from the top elevation array is for visualization. When a MODFLOW solution is displayed in side view, GMS plots the computed water table on top of the cross section display. Using the top elevation of layer 1 as the ground surface makes it possible to see exactly where the water table lies in relation to the ground surface and illustrates where cells are flooded.

HTOP and Thickness Arrays

Part of the input to the Basic Transport package is a set of arrays defining the layer geometry. These arrays include an HTOP array that defines the top elevations for the top layer and a thickness array for each layer. Since MT3DMS can only be used in combination with the True Layer approach in MODFLOW, there is no need to input these arrays in the MT3DMS interface. By default, the HTOP array is assumed to be equal to the top elevation array for layer 1 defined in the Global Options package of MODFLOW. Furthermore, the thickness arrays are automatically generated by GMS using the top and bottom elevation arrays when the Basic Transport package file is written.

ICBUND

The ICBUND button in the Basic Transport Package dialog is used to enter the values of the ICBUND array.

Porosity

The array defining the porosity of each cell in the model can be defined and edited by selecting the **Porosity** button in the Basic Transport Package. This array can also be initialized using a conceptual model in the Map module. It can also be edited on a cell-by-cell basis using the ***Cell Properties*** command.

ICBUND Array

The **ICBUND** button in the Basic Transport Package dialog is used to enter the values of the ICBUND array. The MODFLOW Array Editor is used to edit the ICBUND array.

Values

The ICBUND array contains a value for each cell in the grid defining the type of the cell as either constant concentration, inactive, or variable concentration.

Constant Concentration

A negative ICBUND value indicates that the cell has a constant concentration. The value of the constant concentration is defined in the starting concentration array described below.

Inactive

An ICBUND value of zero indicates that the cell is inactive.

Variable Concentration

A positive ICBUND value indicates that the cell has a variable concentration (i.e., the concentration will be computed as part of the simulation).

Initializing the ICBUND Array

The IBOUND array used by MODFLOW is similar (but not identical) to the ICBUND array. When a new MT3DMS simulation is initialized, the MODFLOW IBOUND array is used to initialize the values of the ICBUND array. Each cell which is designated as inactive in the IBOUND array is designated as inactive in the ICBUND array. Each cell which is designated as active (variable head) in the IBOUND array is designated as active (variable concentration) in the ICBUND array. Each cell that is designated as constant head in the IBOUND array is NOT designated as constant concentration in the ICBUND array. Rather, constant head cells are designated as active (variable concentration) in the ICBUND array.

Cell Attributes Command

In addition to directly editing the ICBUND array, another method for editing the ICBUND array is to select a set of cells and use the ***Cell Properties*** command in the *MT3D* menu.

Activate Cells in Coverage Command

If the ***Activate Cells in Coverage*** command in the Map module is used to change the active/inactive status of the cells, both the IBOUND and ICBUND arrays are updated accordingly.

Flow vs. Transport Inactive Zones

Since the computational domain of the transport simulation does not necessarily have to match the domain of the flow simulation, the active/inactive zones of the ICBUND array may differ from the active/inactive zones of the IBOUND array. In some cases, the active zone for a transport simulation is only a subset of the active zone of the flow simulation. Care should be taken, however, to ensure that any cells defined as inactive in the flow simulation are not defined as active in the transport simulation.

IBOUND vs. ICBUND Display

If a cell is designated as inactive, it is hidden when the grid is displayed, unless the Inactive cells option is selected in the *3D Grid Display Options* dialog, in which case the inactive cells are displayed, but in a different color. If neither MODFLOW nor MT3DMS is in memory, the default 3D grid active/inactive flags are used to control the display of the grid. If MODFLOW is in memory, the active/inactive status of the cells as defined by the IBOUND array is used to display the grid. If both MODFLOW and MT3DMS are in memory, the ICBUND array takes precedence and is used to display the grid.

MT3D Source/Sink Mixing Package

The *Source/Sink Mixing Package* dialog is used to assign concentrations to point sources/sinks (wells, river/streams, specified head, general head) and areal sources/sinks (recharge, evapotranspiration). In most cases, the concentration is assigned to the incoming water when the sources/sinks are acting in the source mode, i.e., contributing water to the system. In sink mode, the concentration of the outgoing water is equal to the concentration of groundwater in the aquifer and the concentrations assigned to the sources/sinks have no effect. The only exception is evapotranspiration. Even though evapotranspiration always acts in sink mode, a concentration can be specified. Generally, the assigned concentration is zero which only allows pure water to leave the aquifer.

Source/Sink Mixing Package dialog

Maximum number of Sources/Sinks in Flow Model

MT3DMS needs to know the maximum number of sources/sinks in the flow model. This number is simply the total number of cells in the MODFLOW model that have a source or sink defined at them. This number is computed automatically.

Point sources/sinks spreadsheet

Values for the concentration as well as the type of source or sink and the location of each of the point source/sink cells are displayed and edited in the spreadsheet. Since the concentration data are time dependent, one value is defined for the concentration at each stress period. Concentration values are displayed in the spreadsheet for the current stress period only. The current stress period is displayed above the spreadsheet and can be changed. If the

concentration values for a previous stress period are the same as those used for the current stress period, the **Use previous** option may be used. When the **Use previous** option is selected, the fields in the spreadsheet cannot be edited.

A column is provided for each of the species concentrations. Changing the source/sink type for one stress period at a cell will automatically change the type for the remainder of the stress periods at the same cell.

Point sources/sinks can be added and removed from the list by selecting the **Add** and **Delete** buttons. However, when adding new point source/sink, it is usually more convenient to select the 3D grid cells and use the ***MT3D\Point Sources/Sinks*** menu command.

Initializing Point Source Sinks from MODFLOW

An option is included in the *Source/Sink Mixing Package* dialog to initialize the point sources/sinks to be used in the MT3DMS simulation directly from data that have already been defined in a MODFLOW simulation. If a MODFLOW simulation is currently in memory, the buttons in the *Initialize point sources/sinks from MODFLOW* dialog can be used. Each button is labeled with a different source/sink type, corresponding to the MODFLOW point sources or sinks. Selecting one of the buttons automatically adds to the list of point sources/sinks. For example, if the Well button is selected, GMS creates a new well source/sink for each cell where a well is defined in the MODFLOW simulation currently in memory. The initial concentration of each of the new well sources/sinks is zero. In order to utilize the source/sink initialization buttons, the following conditions must be met:

1. The MODFLOW package corresponding to the source/sink type to be initialized must have been selected in the MODFLOW Packages dialog.
2. Point sources or sinks of the type to be initialized must have been defined in MODFLOW.

Specified Concentration Boundary Conditions

When entering the concentrations for a specified concentration cell, it is sometimes necessary to specify the concentrations of some of the species but allow the concentrations for the remaining species to vary. This can be accomplished by specifying a negative concentration for the species that are to vary.

Areal Sources/Sinks

Recharge and evapotranspiration are known as areally distributed sources and sinks. This is because a value for concentration must be entered for each species for every vertical column of cells in the finite difference grid. This essentially means that a two dimensional array of concentration values must be defined for each species for both recharge and evapotranspiration, depending upon which options are utilized. The buttons labeled Recharge and Evapotranspiration bring up the Areal Source/Sink Array dialog.

Reset

The Reset button deletes all of the data currently defined in the *Source/Sink Mixing package* and restores the package parameters to the default values.

Conceptual Model Input

In some cases, the simplest way to define both point and areal sources/sinks is with an MT3DMS conceptual model in the Map module. Concentrations can be assigned directly to points, arcs, and polygons; points representing point sources/sinks and polygons representing recharge and evapotranspiration zones. These concentrations are copied directly to the appropriate cells/arrays in the *Source/Sink Mixing package* when the conceptual model is converted to the numerical model with the ***Feature Objects | Map -> MT3DMS*** command.

MT3D point Sources/Sinks BC

The *Source/Sink Mixing Package* dialog can be used to edit both point and areal sources/sinks using a spreadsheet. In many cases, it is more convenient to view and edit source sink concentrations on a cell-by-cell basis. Two commands are provided to facilitate this type of editing: the ***Point Sources/Sinks*** command and the ***Areal Sources/Sinks*** command.

Point Sources/Sinks

The ***Point Sources/Sinks*** command is used to assign and edit the concentrations at point sources and sinks. Before selecting the ***Point Sources/Sinks*** command, a set of cells should be selected using the cell selection tools. Once the command is selected, the *MT3DMS Point Source/Sink* dialog appears.

A point source/sink concentration for each species is assigned to the selected cells by selecting the toggle corresponding to the type of source/sink. The concentration at the cells can be specified as either constant or transient. If a constant value is specified, this number will be used for all stress periods. If the Variable option is used, clicking on the window brings up the XY Series Editor. The XY Series Editor is used to assign a concentration value for each stress period.

Multiple Sources/Sinks per Cell

In many cases, multiple point sources/sinks, each having a different type, can be assigned to an individual cell. In this case, the toggle for each type should be selected and the concentration specified. It is also possible for multiple sources/sinks of the same type to be assigned to a single cell. However, MT3DMS only allows one concentration to be assigned to each type for a single cell. In such cases, the specified concentration for that type applies to all sources/sinks of that type within the cell.

Fixing Concentrations for Selected Species

When entering the concentrations for a specified concentration cell, it is sometimes necessary to specify the concentrations of some of the species but allow the concentrations for the remaining species to vary. This can be accomplished by specifying a negative concentration for the species that are to vary.

Areal Sources/Sinks

The ***Areal Sources/Sinks*** command is used to edit the concentrations assigned to recharge and evapotranspiration fluxes. Before selecting the ***Areal Sources/Sinks*** command, a set of cells should be selected using the cell selection tools. The concentration fluxes due to recharge and evapotranspiration are applied to vertical columns rather than to individual cells. Therefore, to edit the value for a vertical column, any cell in the column can be selected. Once the ***Areal Sources/Sinks*** command is selected, the *MT3DMS Areal Sources/Sinks* dialog appears.

The areal source/sink concentration values at the selected cells can be edited by highlighting a species and either selecting a constant value for all stress periods, or by defining a set of values.

Building an MT3DMS Simulation

Setting up an MT3DMS simulation involves taking a pre-defined MODFLOW simulation and defining some additional properties such as porosity, assigning concentrations to sources and sinks, and choosing some general simulation options. MODFLOW automatically generates a head and flow file (*.hff) containing information on computed heads and fluxes. This file is used as part of the input to the transport model when MT3DMS is launched. MT3DMS uses the top and bottom grid elevation specified in the *Global Options/Basic Package* Dialog. A MODFLOW model must exist in the GMS project prior to creating an MT3DMS simulation.

Two basic approaches are provided in GMS for defining these data: using the 3D Grid module or using the Map module.

Using the 3D Grid Module

Although it is not always the most efficient approach, an MT3DMS simulation can be completely defined using only the tools in the 3D Grid module. With this approach, the material properties and concentrations at sources/sinks are assigned directly to the cells.

Using the Map Module (MT3DMS Conceptual Model)

For sites with complicated boundary conditions and sources/sinks, the preferred method for setting up an MT3DMS simulation is to use the feature object tools in the Map module to define an MT3DMS conceptual model of a site being studied.

In order to use the conceptual model approach to build a MT3DMS model, the same conceptual model must be used for both the MODFLOW flow model and the MT3DMS transport model. This ensures that there is a proper linkage between the sources/sinks in the conceptual model and the sources/sinks in the grid model.

The conceptual model is a high-level description of the site describing sources/sinks, the boundary of the domain to be modeled, recharge and evapotranspiration zones, and material zones within each of the layers. In addition to the parameters required by MODFLOW, many of the parameters required by MT3DMS such as concentrations at sources/sinks and layer data, including porosity and dispersion coefficients, can be assigned directly to the feature objects.

The following steps are used in setting up a conceptual model and converting the conceptual model to a numerical model:

1. Construct a MODFLOW conceptual model, create a grid, and convert the conceptual model data to the MODFLOW data defined at the grid cells.
2. Run the MODFLOW simulation to save the MT3DMS head and flow file.
3. Return to the Map module. Edit the properties of the Conceptual model to include transport. Assign concentrations to the sources/sinks in the conceptual model where necessary. Also define polygonal zones describing layer data including porosity, longitudinal dispersivity, sorption constants, rate constants, and bulk density.
4. Select the ***Feature Objects | Map -> MT3DMS*** command to automatically assign the MT3DMS data to the appropriate cells in the grid.

Saving an MT3DMS Simulation

Once an MT3DMS simulation has been created and checked for potential problems with the Model Checker, the final step is to save the simulation to disk and run MT3DMS. MT3DMS simulations are saved using the ***Save*** and ***Save As*** commands in the ***File*** menu.

Selecting the Save command saves the GMS project including the model simulation. By default the model simulation will be saved to the same location as the GMS project. However, in the Save dialog the path for the model simulation can be specified to be different from the project file if the "Match model names with project name" toggle is unchecked. This is done with the Browse buttons next to each model.

An MT3DMS simulation is saved to a set of input files. The MT3DMS super file is a special type of file which is used to organize the set of files used in a simulation. The names of all of the input and output files associated with a simulation are saved in the super file. When MT3DMS is launched, the name of the super file is automatically passed to the MT3DMS executable.

When an MT3DMS simulation is saved, the names of the other MT3DMS input files are automatically patterned after the name of the super file. For example, if the super file is named sampmod.mts, the other files are named sampmod.btn, sampmod.ssm, etc.

This content also applies to RT3D, SEAM3D and PHT3D.

Importing an MT3D Simulation

It is often necessary to import an MT3DMS simulation that was not generated by GMS. Since GMS uses the standard MT3DMS file format, this is not a problem in most cases. However, there are a few steps and precautions that should be taken.

File Formats

GMS uses the standard MT3DMS file formats described in the MT3DMS documentation (Zheng, 1998). The files you are importing must match these formats exactly. If the files were generated for a version of MT3DMS that uses a different set of file formats, the files will need to be edited before they can be successfully imported to GMS.

CON File

The source code of MT3DMS was changed to create a *.con file instead of the default *.ucn file. GMS can read either the *.con or *.ucn file. The *.con file is written in the GMS binary data set format.

Importing Super Files

GMS uses an MT3DMS super file to organize the files used by an MT3DMS simulation. This file is not a standard MT3DMS file. One approach to importing an externally defined simulation is to create an MT3DMS super file containing the names of the files used in the simulation using a text editor.

MT3DMS Display Options

The properties of all MT3DMS data that GMS displays on the screen can be controlled through the MT3D tab of the *Display Options* dialog. This dialog is opened by right clicking on the 3D Grid Data entry in the Project Explorer and selecting the Display Options command. It can also be accessed from the from the *Display* menu, the *MT3D* menu, or the **Display Options** macro. The following table describes the display options available for the 3D Grid module.

Display Option	Description
Point Sources/Sinks, NAPL Point Sources/Sinks, Constant concentration	The three items at the top of the dialog represent display options for the constant concentration cells and the point sources/sinks. If the check box just to the left of one of these is selected, a symbol is displayed at the center of each cell where that object has been defined. The symbol for each object is displayed in a window to the left of the check box. The symbol can be changed by clicking on the button. This brings up the *Symbol Editor* dialog. The Symbol Editor contains a list of available symbols and can be used to edit the size and color of the symbol.
Display symbol legend	If the Symbol legend option is selected, a legend showing each of the symbols associated with sources/sinks and constant concentration cells is displayed in the lower right corner of the GMS window.
Check All	By clicking this button, all of the display options are turned on.
Check None	By clicking this button, all of the display options are turned off.

Calculate Mass

The *MT3D Calculate Mass* dialog allows the calculation of the mass of a contaminant in the entire model domain or in the selected cells.

Definition

Explains the formula that is used to calculate the mass. Basically, the volume of water in each cell is calculated and then multiplied by the concentration computed by MT3D. A conversion factor must be supplied so that the calculated mass will be computed in the correct units.

Concentration Range

Allows the specification a range over which the mass will be calculated. This is most useful to ignore negative concentrations that result in MT3D simulations.

Conversion Factor

The factor determines which units the resulting mass will be displayed in.

MT3D Commands

Menu Command	Description
New Simulation...	
Delete Simulation...	
Check Simulation...	
Run Options...	
Run RT3D...	
Read Solution...	
Display Options...	
Point Sources/Sinks...	
Areal Sources/Sinks...	
Cell Properties...	
Calculate Mass...	
Basic Transport Package...	
Advection Package...	
Dispersion Package...	
Source/Sink Mixing Package...	
Chemical Reaction Package...	
Transport Observation Package...	
GCG Package...	
Biodegradation Package...	
NAPL Dissolution Package...	
Reductive Dechlorination Package...	
Cometabolism Package...	

6.6. PEST

PEST

PEST is a general purpose parameter estimation utility developed by John Doherty of Watermark Computing. The PEST interface in GMS can be used to perform automated parameter estimation for MODFLOW. The steps involved in setting up a PEST run are described in the automated parameter estimation topic.

The PEST options are edited by selecting the ***Parameter Estimation*** command in the *MODFLOW* menu and then clicking on the PEST tab.

PEST version support

The following table shows the version of PEST supported by different versions of GMS. To see the latest released version of PEST visit http://www.pesthomepage.org/Downloads.php.

GMS	PEST
GMS 6.5	PEST 10.0
GMS 7.0	PEST 10.0
GMS 7.1	PEST 12.0
GMS 8.0, 8.1, 8.2	PEST 12.1
GMS 8.3, 9.0	PEST 12.2
GMS 9.1	PEST 12.3

6.7. PHT3D

PHT3D

PHT3D	
Model Info	
Model type	geochemical, multi-species reactive transport
Developer	Henning Prommer, Vicent Post
Documentation	PHT3D website [1] PHT3D Manual [2]
Tutorials	GMS:Tutorials

PHT3D is a multicomponent transport model for three-dimensional reactive transport in saturated porous media developed and maintained by Henning Prommer and Vicent Post. PHT3D is a combination of MT3DMS and PHREEQC-2. The PHREEQC component allows for a variety of low temperature aqueous geochemical reactions.

Basic Transport Package

To use PHT3D, the user selects *PHT3D* as the Model in the *Basic Transport Package* dialog.

Define Species

The options that are specific to PHT3D are entered when defining the species for the simulation. When the **Define Species** button is selected the *PHT3D Options* dialog comes up. In addition to defining the species for the simulation, the user can enter options specific to PHT3D (such as temperature, activation criterion etc.) See the PHT3D documentation for more information on specific variables in this dialog.

PHT3D requires as part of its input a PHREEQC database file. The species that can be included in the simulation depend on the contents of the PHREEQC database file. The browser button near the top of the *PHT3D Options* dialog allows the user to select a PHREEQC database file. GMS will parse the contents of this file and make available the species listed in the file. The user also has the option to select a PHT3D-PHREEQC interface file. When an interface package file is chosen GMS assumes that the PHREEQC database file is in the same directory with the name pht3d_datab.dat. In addition to parsing the PHREEQC database, the interface file is also read and any options that are specific to the species are imported.

The PHREEQC database file can contain many species. When a user is only using a small subset of the available species in the database it is useful to only show the species that are active (in use). The **Only show active species** check box hides all of the species that are not active.

All other inputs to PHT3D are the same as MT3DMS. For more information on how to use PHT3D the user is referred to the GMS tutorials.

References

[1] http://pht3d.org

[2] http://gmsdocs.aquaveo.com/PHT3D_manual_v210.pdf

6.8. RT3D

RT3D

RT3D	
Model Info	
Model type	multi-species reactive transport
Developer	Battelle Pacific Northwest National Laboratory
Documentation	RT3D Manual v1 [1] RT3D Manual v2.5 [2]
Tutorials	RT3D Tutorials

RT3D is a multi-species reactive transport model developed by the Battelle Pacific Northwest National Laboratory. RT3D is a modified version of MT3DMS that utilizes alternate Chemical Reaction packages. Numerous pre-defined reactions are available and an option is provided for creating user-defined reactions. RT3D is well-suited for simulating natural attenuation and bioremediation.

Since RT3D is a modified version of MT3DMS, most of the input to RT3D is identical to the input required for MT3DMS. Thus, the RT3D interface is contained within the *MT3D* menu in the 3D Grid module. In the *Basic Transport Package* dialog, an option is provided for selecting the current model as either MT3DMS, RT3D, or SEAM3D. A number of options in the interface then change based on which model is selected.

Since much of the RT3D interface is identical to the MT3DMS Interface, only the portions of the interface which are unique to RT3D are described in this help file.

Basic Transport Package

The first step in defining an RT3D simulation is to define the data required by the Basic Transport (BTN) package. The options in the *Basic Transport Package* dialog unique to RT3D are as follows:

Packages

The Packages button brings up the *Packages* dialog. If the RT3D model is the current model and the Chemical Reaction package is selected, one of the RT3D reactions must be selected from the pull-down list. The first nine reactions are pre-defined reaction types. If one of these reactions is selected, the names of the species and the names of the reaction parameters are automatically determined by GMS. The last reaction is a user-defined reaction. If this option is selected, a list of species and list of reaction parameters must be specified by the user.

Define Species

For most of the reaction package options, once the reaction package is selected, the list of species used by the package is automatically initialized by GMS. However, if the user-defined reaction package is selected, the **Define Species** button is undimmed in the *Basic Transport Package* dialog and a list of species must be manually defined before any concentrations are assigned to sources/sinks.

Chemical Reactions Package

The Chemical Reactions Package dialog utilized by RT3D is different from the MT3DMS Chemical Reactions dialog. The items in the dialog unique to RT3D are as follows:

Solver

If the selected reaction package is a kinetic reaction, several solvers are available for the solution of the chemical reaction equations. The desired solver should be selected from the Solver pull-down list. When one of these solvers is used, an absolute and relative tolerance must be specified for each of the mobile species using the atol and rtol parameters.

Reaction Parameters

With each reaction package, a set of reaction parameters must be defined. The method used to edit the reaction parameters depends on whether the reaction is a pre-defined reaction or a user-defined reaction.

Pre-Defined Reactions

For the pre-defined reactions, the number of reaction parameters and the names of the parameters are fixed. If the Spatially vary all toggle is off, a single value is entered for each parameter using the edit field below the parameter list. If the **Spatially vary all** toggle is on, an array of values is entered for each parameter using the **Edit** button. In this case, the cell-by-cell parameter values can also be edited using the ***Cell Attributes*** command.

User-Defined Reactions

For user-defined reactions, the list of reaction parameters must be defined using the **Define Parameters** button. This button brings up the Define Parameters dialog. This dialog functions similarly to the *Define Species* dialog. The New and Delete buttons are used to add and remove items from the list. The **Import** button is used to read a previously defined list of reaction parameters from an RT3D super file (*.rts).

With the pre-defined reactions, the reaction parameters are either all spatially variable or all constant. However, with the user-defined reaction option, selected parameters may be designated as spatially variable while others are designated as constant. The variable/constant status of a parameter is selected using the Spatially variable toggle in the *Define Parameters* dialog.

References

[1] http://gmsdocs.aquaveo.com/rt3dman.pdf
[2] http://gmsdocs.aquaveo.com/rt3dv2.5man.pdf

Basic Transport Package Dialog

The first step in setting up an MT3DMS simulation is to define the data for the Basic Transport package. The information defined in the Basic Transport package includes the computational time intervals (stress periods), an array defining which cells are inactive and which cells have constant concentration, an array defining aquifer porosity, and array of starting concentration values. The input data for the Basic Transport package must be entered before editing any of the other packages in the MT3DMS simulation. The *Basic Transport Package* dialog contains the following options:

Headings

A brief description of the model can be entered in the two lines provided at the top of the Basic Transport Package dialog. This information is printed to the ASCII listing file output by MT3DMS.

Model Selection

The Model section in the middle of the *Basic Transport Package* dialog is used to select which transport model is to be used. The menu commands and packages and options that are available depend on which model is selected. All MT3D-based transport models are contained in the *MT3D* menu. See the RT3D, SEAM3D and PHT3D pages for more information on those transport models.

Stress Periods

As is the case with MODFLOW, the computational time intervals for an MT3DMS simulation are called "stress periods". Concentrations at boundary conditions or source/sink terms can only change at the beginning of each stress period. Stress periods are subdivided into time steps and time steps are subdivided into transport steps. The **Stress Periods** button on the left of the *Basic Transport Package* dialog is used to bring up the *Stress Period* dialog. If a transient MODFLOW simulation is used, the stress periods and time steps used for MT3DMS are initialized to coincide exactly with those defined for MODFLOW. If a steady state MODFLOW simulation is used, any set of stress periods may be utilized for MT3DMS.

The *Stress Periods* dialog is identical to the *MODFLOW Stress Periods* dialog except for two fields. In addition to the stress period definition required by MODFLOW, MT3DMS also requires a transport step size and a maximum number of transport steps allowed for one time step. These values are defined for each stress period. If a value of zero is entered for the transport step size (the default), MT3DMS will automatically calculate an appropriate transport step size. Furthermore, if the value for the transport step size entered by the user is larger than the value computed by MT3DMS, the MT3DMS value will be used. The transport step size times the Max transport steps must be longer than the total simulation length.

Output Control

Options for printing and saving the results from an MT3DMS simulation are also included in the Basic Transport package. The MT3DMS output control options are modified by selecting the Output Control button on the left side of the *Basic Transport Package* dialog. This brings up the *MT3D Output Control* dialog.

One of the output options is an unformatted (binary) concentration file which is used for post-processing by GMS. This option is selected using the toggle at the bottom of the dialog. With the version of MT3DMS included with GMS, the concentration file is saved directly from MT3DMS as a GMS binary scalar data set file.

Another option is to Print or save at specified times. When this option is selected, the Times button is undimmed. Selecting the **Times** button brings up a spreadsheet that enables users to specify the times that the output will be printed or saved. The spreadsheet can be quickly initialized by selecting the **Initialize Values** button at the bottom of

the dialog. This button brings up the *Initialize Time Steps* dialog. This dialog is composed of edit fields that will automatically populate the times that MT3D data will be saved or printed.

Packages

The **Packages** button on the left of the Basic Transport Package dialog brings up the *Packages* dialog. This dialog is used to specify which of the packages are to be used in the simulation. The check box to the left of the package name is selected to signify that a package will be utilized as part of the simulation. Some of the packages are used by RT3D or SEAM3D and are dimmed for MT3DMS simulations.

Define Species

MT3DMS is a multi-species transport model. It can track the migration and concentration of several species at once. The **Define Species** button is used to define the number of species in the simulation and the name and type of each species. The button brings up the *Define Species* dialog.

The species are listed in the box on the left side of the dialog. Species are added and deleted using the **New** and **Delete** buttons. The name of a selected species can be edited. The **Mobile** toggle is used for RT3D and is dimmed for MT3DMS simulations.

The species names are not used by the MT3DMS code. They are only used in GMS to simplify the model input. In MT3DMS, all species are identified by an integer ID. The species names are saved to the MT3DMS super file (*.mts). When building a new simulation, it is sometimes useful to use the same set of names used in a previous simulation. This can be accomplished by selecting the Import button and selecting the MT3DMS super file used by the previous simulation. This automatically loads in the species names to the list.

Units

All MT3DMS input parameters must be entered using a consistent set of units. The Units button brings up a dialog which can be used to specify a standard unit for length, time, mass, force, and concentration. The selected units are used by GMS to post the appropriate unit labels next to each of the input fields in the MT3DMS interface. These labels serve as a reminder to the user of the correct units. The units must be consistent with the units used in the MODFLOW simulation.

CINACT

The CINACT value is written to the MT3DMS solution file wherever an inactive concentration cell exists (ICBUND=0). This value should be selected so that it will not likely be a valid concentration computed from MT3DMS. The default value of -999 is generally sufficient.

Use Materials for Porosity and Long. Dispersivity

If this option is selected, the porosities and longitudinal dispersivities specified in the Materials dialog will be used in the MT3DMS model.

HTOP Equals Top of Layer 1

In some cases it is useful to explicitly define the HTOP array separately from the top elevation array for layer 1 defined in the Global Options package. If the toggle entitled HTOP equals top of layer 1 is turned off, an HTOP array can be explicitly defined. This option should be used if the top of layer 1 is substantially higher than the computed water table. In such cases, using the top of layer 1 could lead to significant error (see MT3DMS Reference Manual).

Another option would be to use the default approach and lower the value of the layer 1 top elevation array. For unconfined layers, this array is not used by MODFLOW anyway. The only reason to keep the HTOP array separate from the top elevation array is for visualization. When a MODFLOW solution is displayed in side view, GMS plots the computed water table on top of the cross section display. Using the top elevation of layer 1 as the ground surface makes it possible to see exactly where the water table lies in relation to the ground surface and illustrates where cells are flooded.

HTOP and Thickness Arrays

Part of the input to the Basic Transport package is a set of arrays defining the layer geometry. These arrays include an HTOP array that defines the top elevations for the top layer and a thickness array for each layer. Since MT3DMS can only be used in combination with the True Layer approach in MODFLOW, there is no need to input these arrays in the MT3DMS interface. By default, the HTOP array is assumed to be equal to the top elevation array for layer 1 defined in the Global Options package of MODFLOW. Furthermore, the thickness arrays are automatically generated by GMS using the top and bottom elevation arrays when the Basic Transport package file is written.

ICBUND

The ICBUND button in the Basic Transport Package dialog is used to enter the values of the ICBUND array.

Porosity

The array defining the porosity of each cell in the model can be defined and edited by selecting the **Porosity** button in the Basic Transport Package. This array can also be initialized using a conceptual model in the Map module. It can also be edited on a cell-by-cell basis using the ***Cell Properties*** command.

6.9. SEAM3D

SEAM3D

SEAM3D	
Model Info	
Model type	reactive transport
Developer	Mark Widdowson at Virginia Tech University
Documentation	SEAM3D Manual [1]
Tutorials	MODAEM Tutorials

SEAM3D is a reactive transport model used to simulate complex biodegradation problems involving multiple substrates and multiple electron acceptors. It is based on the MT3DMS code. In addition to the regular MT3DMS modules, SEAM3D includes a Biodegradation package and NAPL Dissolution package. SEAM3D was developed by Mark Widdowson at Virginia Tech University.

Since SEAM3D is a modified version of MT3DMS, most of the input to SEAM3D is identical to the input required for MT3DMS. Thus, the SEAM3D interface is contained within the MT3D menu in the 3D Grid module. In the *Basic Transport Package* Dialog, an option is provided for selecting the current model as either MT3DMS, RT3D, or SEAM3D. A number of options in the interface then change based on which model is selected.

References

[1] http://gmsdocs.aquaveo.com/SEAM3Dv3.pdf

6.10. SEAWAT

SEAWAT

SEAWAT	
Model Info	
Model type	3D Flow and Transport Model
Developer	USGS
Documentation	SEAWAT Manual [1]
Tutorials	SEAWAT Tutorials

SEAWAT is a three dimensional variable density groundwater flow and transport model developed by the USGS based on MODFLOW and MT3DMS. SEAWAT v4 is based on MODFLOW 2000 and MT3DMS 5.2. SEAWAT includes two additional packages: Variable-Density Flow (VDF) and Viscosity (VSC). A complete description of SEAWAT is beyond the scope of this reference manual. It is assumed that the reader has a basic knowledge of SEAWAT and has read the SEAWAT documentation.

GMS supports SEAWAT as a pre- and post-processor. The interface to SEAWAT relies on the interface to MODFLOW and MT3DMS. The input data for SEAWAT is generated by GMS and saved to a set of files including a MODFLOW model, an MT3D model if transport is used, and a SEAWAT model pointing to the MODFLOW and MT3D model's package files. These files are then read by SEAWAT and executed. SEAWAT uses the MODFLOW and MT3D interfaces for boundary condition display and for post-processing.

SEAWAT Links

- Building a SEAWAT Model
- SEAWAT Global Options Dialog
- SEAWAT MODFLOW AUX Variables
- SEAWAT Packages
- Importing a SEAWAT Simulation
- MODFLOW with HDF5

References

[1] http://gmsdocs.aquaveo.com/seawatv4.pdf

Building a SEAWAT Model

SEAWAT	
Model Info	
Model type	3D Flow and Transport Model
Developer	USGS
Documentation	SEAWAT Manual [1]
Tutorials	SEAWAT Tutorials

Grid Approach

Although it is not always the most efficient approach, a SEAWAT simulation can be completely defined using only the tools in the 3D Grid module. To build a SEAWAT model with this approach you must first create a MODFLOW model using the grid approach. If using transport, an MT3D model is then created, and then a SEAWAT model is created. For each of the 3 models the properties and concentrations at sources/sinks assigned directly to the cells. Any SEAWAT MODFLOW AUX Variables are assigned using the MODFLOW package dialogs. SEAWAT specific packages can be set using the VDF or VSC package dialogs.

Conceptual Model Approach

To create a SEAWAT using a conceptual model:

1. Construct a MODFLOW conceptual model, create a grid, and convert the conceptual model data to the MODFLOW data defined at the grid cells.
2. Run the MODFLOW simulation to make sure it is working properly.
3. If the simulation includes transport, return to the Map module. Edit the properties of the Conceptual model to include transport. Assign concentrations to the sources/sinks in the conceptual model where necessary. Also define polygonal zones describing layer data including porosity, longitudinal dispersivity, sorption constants, rate constants, and bulk density.
4. Select the *Feature Objects | Map -> MT3DMS* command to automatically assign the MT3DMS data to the appropriate cells in the grid.
5. Enable SEAWAT in the MODEL interfaces dialog and create a SEAWAT simulation.
6. Edit the MODFLOW AUX variables, VDF, and VSC packages if necessary.
7. Use the SEAWAT model checker to check the simulation for any errors or warnings.

SEAWAT Global Options Dialog

SEAWAT	
Model Info	
Model type	3D Flow and Transport Model
Developer	USGS
Documentation	SEAWAT Manual [1]
Tutorials	SEAWAT Tutorials

The *Global Options* Dialog is used to setup a new SEAWAT model or to edit the current options for an existing model. To set up a new SEAWAT model select Edit|Model Interfaces... menu and turn on the SEAWAT model interface. Next select SEAWAT|New menu item to create the SEAWAT model.

In the Global Options dialog, toggles are provided to modify the use of transport in the simulation, to turn on and off the Variable-Density Flow (VDF) and Viscosity (VSC) packages, and to enable or disable the SEAWAT MODFLOW AUX Variables variables used by SEAWAT.

SEAWAT MODFLOW AUX Variables

SEAWAT	
Model Info	
Model type	3D Flow and Transport Model
Developer	USGS
Documentation	SEAWAT Manual [1]
Tutorials	SEAWAT Tutorials

SEAWAT allows using MODFLOW AUX variables for some packages to set values used for MODFLOW packages the variables include:

- WELDENS - Density of well fluid (WEL package).
- DRNBELEV - Drain bottom elevation (DRN package).
- RBDTHK - River bed thickness (RIV package).
- RIVDEN - Density of river fluid (RIV package).
- GHBELEV - General head elevation (GHB package).
- GHBDENS - Density of general head fluid (GHB package).
- CHDDENSOPT and CHDDEN - Constant head fluid density (CHD package).

These AUX variables can be enabled by selecting them in the SEAWAT Global Options Dialog and can be edited in the associated MODFLOW package dialog or in the MODFLOW Sources/Sinks dialog.

SEAWAT Packages

SEAWAT	
Model Info	
Model type	3D Flow and Transport Model
Developer	USGS
Documentation	SEAWAT Manual [1]
Tutorials	SEAWAT Tutorials

SEAWAT specific packages include the Variable-Density Flow (VDF) and Viscosity (VSC) packages. The package dialogs for both packages are available under the SEAWAT menu. For the package menu items to be available, the packages must first be enabled from the SEAWAT Global Options Dialog. For a detailed description of the VDF and VSC input options, please refer to the SEAWAT manual available in the side bar.

VDF Package

The VDF package can be used in a SEAWAT simulation to model the affects of concentration on fluid density. The input values available in the VDF package include:

- IWTABLE - Active variable-density water table corrections.
- MFNADVFD - Internodal density calculation method.
- DENSEMIN - Minimum fluid density.
- DENSEMAX - Maximum fluid density.
- FIRSTDT - Length of first transport time step.
- NSWTCPL - Flow/transport coupling.
- DNSCRIT - Convergence criteria.
- MT3DRHOFLG - type of fluid density calculation.
  - When equal to zero, the fluid density for each grid cell can be entered in the table at the bottom of the dialog. For INDENSE enter -1 to use values from previous stress period, 0 to use DENSREF, and 1 to enter values for DENSE column.
  - When equal to -1, the fluid density will be calculated using one or more species entered in the table at the bottom of the dialog using species ID, DRHODC, and CRHOREF. Rows can be entered into the table with the tool bar below the table.
  - When greater than or equal to 1 density is calculated using the corresponding species number.
- DENSREF - Reference fluid density.
- DRHODC - Density/conc. slope.
- DRHODPRHD - Density/pressure slope.
- PRHDREF - Reference pressure head.

VSC Package

The VSC package can be used in a SEAWAT simulation to model the affects of concentration on fluid viscosity. Using the Viscosity Package requires using the VDF package and the LPF package in MODFLOW. The input values available in the VSC package include:

- VISCMIN - Minimum viscosity.
- VISCMAX - Maximum viscosity.
- MT3DMUFLG - Type of viscosity calculation.
  - When equal to zero, the fluid viscosity for each grid cell can be entered in the table at the bottom of the dialog. For INVISC enter -1 to use values from previous stress period, 0 to use VISCREF, and 1 to enter values for VISC column.
  - When equal to -1, the fluid density will be calculated using one or more species entered in the table at the bottom of the dialog using species ID, DMUDC, and CMUREF. Rows can be entered into the table with the tools bar below the table.
  - When greater than or equal to 1 viscosity is calculated using the corresponding species number.
- VISCREF - Reference viscosity.
- DMUDC - Viscosity/concentration slope.
- CMUREF - Reference concentration.
- MTMUTEMPSEC - Temp. species ID.
- AMUCOEFF - coefficients for equation 18-20 in SEAWAT 4 documentation.

SEAWAT Importing a SEAWAT Simulation

SEAWAT	
Model Info	
Model type	3D Flow and Transport Model
Developer	USGS
Documentation	SEAWAT Manual [1]
Tutorials	SEAWAT Tutorials

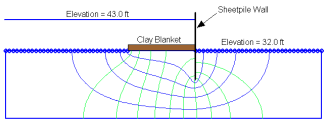
An existing SEAWAT v4 model can be imported into GMS by opening the name file which must have a "*.nam" extension. Upon opening the name file GMS uses the name file to determine if the simulation is MODFLOW-2000, MODFLOW-2005, or a SEAWAT simulation based on the packages included. Once the import is complete, if the model includes transport packages or the VDF or VSC packages then a SEAWAT model is automatically created inside GMS. If the model only includes MODFLOW packages, then the SEAWAT model needs to be created by enabling the SEAWAT model interface by selecting SEAWAT in the Model Interfaces dialog available under the Edit menu, and then selecting ***New Simulation*** under the *SEAWAT* menu.

SEAWAT Commands

Menu Command	Description
New Simulation...	
Delete Simulation...	
Check Simulation...	
Run SEAWAT...	
Read Solution...	
VDF Package...	
VSC Package...	

6.11. SEEP2D

SEEP2D

SEEP2D	
Sample Confined Seepage Problem  *SEEP2D Screenshot*	
Model Info	
Model type	2D seepage, confined or unconfined, steady state
Developer	Fred Tracy, ERDC [1]
Documentation	SEEP2D Primer [2]
Tutorials	SEEP2D Tutorials

SEEP2D is a two-dimensional steady state finite element groundwater model developed by Fred Tracy of the Engineer Research and Development Center [1]. Both saturated and unsaturated flow is simulated. SEEP2D is designed to be used on profile models (XZ models) such as cross-sections of earth dams or levees.

A variety of options are provided in GMS for displaying SEEP2D results. Contours of total head (equipotential lines) and flow vectors can be plotted. An option is also available for computing flow potential values at the nodes. These values can be used to plot flow lines. Together with the equipotential lines (lines of constant total head), the flow lines can be used to plot a flow net. The phreatic surface can also be displayed.

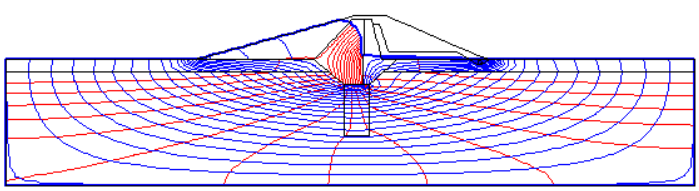
A more complete description of the SEEP2D model, including a discussion of boundary conditions and guidelines for model conceptualization is contained in the SEEP2D Primer. The SEEP2D Primer should be reviewed before consulting this help file. The user is also encouraged to complete the SEEP2D tutorials.

Portions of a SEEP2D model can be imported from GeoStudio files.

Building a SEEP2D Simulation

For a typical application, the following steps are used to perform a SEEP2D simulation using GMS:

1. **Generate a 2D mesh** - The first step in setting up a SEEP2D simulation is to construct a 2D finite element mesh. This can be accomplished using the ***Feature Objects | Map -> 2D Mesh*** command in the Map module. SEEP2D only supports



Sample flow net from SEEP2D

meshes composed entirely of linear elements (three node triangles and four node quadrilaterals). The mesh should not contain quadratic elements (six node triangles and eight node quadrilaterals).

2. **Select the analysis options** - The analysis options are used to set up the type of problem being modeled and to defined constants that are used by SEEP2D when calculating the solution. The items in the dialog are as follows:
   - *Title* - A descriptive title can be entered for the simulation. This title is used in the header of the SEEP2D input and output files. It can also be displayed at the top of the Graphics Window in GMS by turning on the **Title** option in the *SEEP2D Display* Options dialog.
   - *Datum* - By default, the datum of the model is at zero, but it can be specified to any convenient value, such as the value corresponding to the base or lowest y coordinate of the model.
   - *Unit Weight of Water* - The unit weight of water must be entered. SEEP2D uses this value to compute pore pressures. The weight and length units defined in this value should be consistent with the units used elsewhere in the model.
   - *Units* - The **Units** button brings up the *Units* dialog. This dialog is used to enter the units for length, time, concentration, etc. for the simulation. GMS uses the selected unit options to display the appropriate units next to each input edit field in the other SEEP2D dialogs.
   - *Problem Type* - The problem type must be specified either as plane flow or axisymmetric flow. The axisymmetric option should be selected for models corresponding to flow to a single well as described in the SEEP2D Primer. All other models should use the plane flow option.
   - *Flow Lines* - If the Compute flow lines option is turned on, once the head solution is computed, SEEP2D will reverse the boundary conditions and compute flow potential values at the nodes. These values can be contoured by GMS using the Flow lines option is the *SEEP2D Display Options* dialog.
   - *Model Type* - The model type should be selected as either Confined or Unconfined. For confined models, the entire model domain is assumed to be saturated. No exit face boundary conditions should be applied and the unsaturated zone material properties are not required. For unconfined models, two options are available for dealing with the unsaturated zone: (1) deforming mesh and (2) saturated/unsaturated flow modeling. For both types of problems, exit face boundary conditions should be applied along the boundary of the mesh where the free surface is expected to exit. With the deforming mesh option, SEEP2D iterates to find the location of the phreatic surface and the mesh is deformed or truncated so that the upper boundary of the mesh matches the phreatic surface. The solution files from this type of simulation include a geometry file containing the deformed mesh. With the saturated/unsaturated option, the mesh is not modified and the flow in both the saturated and unsaturated zone is modeled. The hydraulic conductivity in the unsaturated zone is modified (reduced) using either the linear frontal method or the Van Genuchten method. The equations used by both methods are described in more detail in the SEEP2D Primer.
3. **Assign the material properties** - Each element in the 2D mesh is assigned a material ID. The material properties are assigned to each element using these IDs and a list of material properties. The material properties specific to SEEP2D are entered using the ***Material Properties*** command in the *SEEP2D* menu. This command brings up the *SEEP2D Material Properties* dialog. The items in the dialog are as follows:
   - *List of Materials* - The currently defined materials are listed at the top of the dialog. The values for a material are entered by selecting the material and editing the values in the lower part of the dialog.
   - *Soil Coefficients* - The hydraulic conductivity in the two major principal directions and the angle from the x-axis to the major principal axis are entered in the Soil Coefficients section. These hydraulic conductivity values represent the hydraulic conductivity for saturated conditions.
   - *Van Genuchten Parameters* - If the Van Genuchten Saturated/Unsaturated option has been selected in the *SEEP2D Analysis Options* dialog, the Van Genuchten alpha and n-value numbers must be defined.
   - *Linear Front Parameters* - If the Saturated/Unsaturated with Linear Front option has been selected in the *SEEP2D Analysis Options* dialog, the minimum pressure head (ho) and minimum relative conductivity (kro) values must be defined.

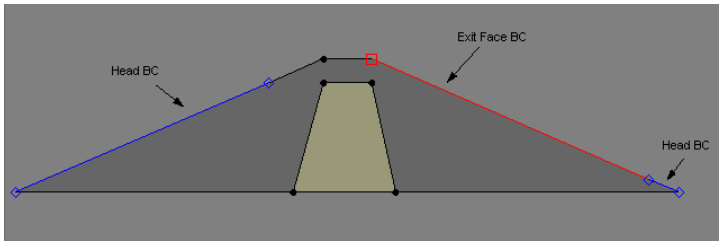
4. **Assign the boundary conditions** (either with a conceptual model or with the 2D mesh tools) - Two general types of boundary conditions can be defined for SEEP2D simulations: nodal boundary conditions and flux boundary conditions. (See SEEP2D Boundary Conditions)
5. **Run the Model Checker.**
6. **Save the simulation**
7. **Run the simulation**
8. **Display the results** - Before reading in the solution file for post-processing in GMS, it is often useful to examine the text output listing file. The output file can also be viewed by simply double-clicking on the *.out file found in the SEEP2D solution folder in the Project Explorer. Also, any text file can be viewed by selecting the ***Edit File*** command in the *File* menu. The File Browser appears and the selected file is opened in a text editor. Once the solution is imported to GMS, a variety of options are available for displaying the solution. The total head and pressure head data sets can be contoured. Velocity vectors corresponding to Darcy velocity can be plotted. If the Compute flow lines option was selected, a complete flow net may be plotted by displaying contours of total head (equipotential lines) and turning on the Flow lines option in the *SEEP2D Display Options* dialog.

SEEP2D Boundary Conditions

Two general types of boundary conditions can be defined for SEEP2D simulations: nodal boundary conditions and flux boundary conditions. The type or value assigned to a previously defined boundary condition can be edited by selecting the node or node string and selecting either the ***Node BC*** or ***Flux BC*** commands. A boundary condition can be deleted by selecting the boundary condition using either the Select Node or Select Node String tools and selecting the ***Delete BC*** command in the *SEEP2D* menu.

Nodal Boundary Conditions

The most common type of SEEP2D boundary conditions is nodal boundary conditions. Nodal boundary conditions are assigned by selecting the nodes and selecting the ***Node BC*** command in the *SEEP2D* menu. When selecting the nodes, either the Select Node tool or the Select Node String tool may be used. The ***Node BC*** command brings up the *Node BC* dialog. Three types of nodal boundary conditions can be assigned: head, exit face, and flow rate.



Sample SEEP2D Problem Showing Boundary Conditions

- **Head BC** - Specified head boundary conditions represent boundaries where the head is known. They typically are found where water is ponding or at the boundary of a region where the water table is known to remain constant. Since the head along such boundaries cannot change, they represent regions of the model where flow enters or exits the system (flow lines are always orthogonal to constant head boundaries).
- **Exit Face BC** - Exit face boundary conditions imply that the head is equal to the elevation (assuming that the datum is 0). They are used when modeling unconfined flow problems and should be placed along the face where the free surface is likely to exit the model. This boundary condition must be used if the option for deforming the mesh to the phreatic surface has been selected in the analysis options. It may also be used with a saturated/unsaturated flow model. In this case, if the head at a node on the boundary becomes greater than the node elevation during the iteration process, the head at the node is fixed at the nodal elevation and the node acts as a specified head boundary. Thus, water is allowed to exit the boundary above the tailwater. If an exit face boundary is not used with a saturated/unsaturated flow model, all of the flow will be forced through the tailwater.

- **Flow Rate BC** - Flow rate boundary conditions are used to specify nodes at which a certain flow rate is known to exist. They are used primarily when modeling wells and the flow specified represents the pumping rate. Negative values represent extraction of fluid from the system whereas positive values represent injection.

Flux Boundary Conditions

Flux boundary conditions are used to specify a known flux rate [L/T] along a sequence of element edges on the perimeter of the mesh. They are often used to simulate infiltration. Flux into the system is positive and flux out of the system is negative.

Flux BC are assigned by selecting a sequence of nodes along the mesh boundary using the Select Node String tool and selecting the ***Flux BC*** command in the *'SEEP2D* menu. This command brings up a simple prompt for the flow rate.

Reading the SEEP2D Solution

Once the simulation is completed, the solution is automatically imported to GMS for post-processing. The solution files are organized in a SEEP2D solution folder in the Project Explorer. If the unconfined/deforming mesh option is selected, the solution will consist of two files: a geometry file that contains the deformed mesh and a solution file that contains the head, velocity, and flow potential data sets. If any of the other analysis options is selected, only the solution file is saved. Regardless of which option is used, the solution can be quickly imported to GMS using the ***Read Solution*** command in the *SEEP2D* menu. The solution data sets are organized into a SEEP2D solution folder in the Data Tree.

SEEP2D Files

See the main page about SEEP2D files at SEEP2D Files.

References

[1] http://www.erdc.usace.army.mil/
[2] http://gmsdocs.aquaveo.com/s2dprimr.pdf

SEEP2D Display Options

The properties of all SEEP2D data that GMS displays on the screen can be controlled through the SEEP2D tab of the *Display Options* dialog. This dialog is opened by right clicking on the 2D Mesh Data entry in the Project Explorer, selecting the ***Display Options*** command, and then selecting the SEEP2D tab. This tab is only visible when there is a SEEP2D simulation. It can also be accessed from the from the ***Display*** menu, the *SEEP2D* menu, or the **Display Options** macro. The following table describes the display options available for the SEEP model.

Display Option	Description
Head BC	The Head BC, Exit face BC, Flux rate BC, and Flux BC items can be used to turn on the display of a symbol for each of the boundary condition types. The color and type of symbol can be edited by clicking on the button to the left of each item.
Exit face BC	
Flow rate BC	
Flux BC	
BC values	If the BC values option is selected, the numerical value of each boundary condition (head, flux rate, etc.) is displayed next to the boundary condition. The font used to display the values can be editing by clicking on the button to the left of the item.
Flow lines	If the Compute flow lines option is selected the SEEP2D Analysis Options dialog prior to saving and running the model, SEEP2D performs the computations in two steps. In the first step, SEEP2D solves for the heads. In the second step, the head solution is used to "reverse" the boundary conditions and a second solution is found. This solution represents "flow potential" values. When the solution is read back into GMS, these flow values can be contoured to generate a plot of flow lines. When superimposed on contours of total head (equipotential lines) a complete flow net can be displayed. (see ***Note***)
Title	If the Title option is selected, the problem title specified in the *Analysis Options* dialog will be displayed at the top of the Graphics Window.
Total flow rate	If the Total flow rate option is selected and if a solution is in memory, the total flow rate through the model will be displayed at the top of the Graphics Window, just below the title.
Phreatic surface	If the Phreatic Surface option is selected and if a solution is in memory, the phreatic surface will be displayed on the mesh. The color and type of line can be edited by clicking on the button to the left of the item.
Check All	By clicking this button, all of the display options are turned on.
Check None	By clicking this button, all of the display options are turned off.

***Note**: When contouring the flow values, GMS must determine a contour interval that will result in the proper number of flow channels. The number of flow channels is computed by solving for numflow in the following equation:*

$$q = k_{\text{equiv}} \frac{\text{numflow}}{\text{numequipotential}} \Delta H$$

The kequiv value is solved for using the k values for the base material specified using the combo box just below the Flow Lines option. The equivalent k is computed as follows:For problems with several material zones where each material is isotropic, the flow net cells in the base material will appear to be square, while the cells in the other material zones will be stretched. The amount of stretching is a function of the relative difference in k values between the material and the base material.

SEEP2D Solution

After a SEEP2D simulation is run in GMS, the solution to this simulation can be automatically loaded into GMS. The solution will appear in the Project Explorer under the 2D Mesh Data folder in its own subfolder. The subfolder will appear with a lock image on it. The image means that the information in the solution folder is locked and cannot be edited from within GMS. The solution datasets in the solution can be contoured and viewed in GMS. The potential datasets that may be part of a SEEP2D solution are listed below. A description of each also follows.

Total Head	the pressure head plus the elevation head (same as the head measured by a piezometer).
Pressure Head	the water pressure divided by the unit weight of water.
Pore Pressure	the hydrostatic pressure.
Flowrate	the flow rate of water into (out of) the problem domain.
Velocity	the discharge velocity is calculated by multiplying the gradient by hydraulic conductivity [k*i]. This is a vector data set and is accompanied by a scalar data set called *velocity_Mag* that is the magnitude of the vector data set.
Gradient	the hydraulic gradient is calculated by dividing the difference in Total Head by distance [$(h_1-h_2)/L$]. This is a vector data set and is accompanied by a scalar data set called *gradient_Mag* that is the magnitude of the vector data set.
Flowline	this data set is used to create a flow net when the Total Head data set is the active data set.

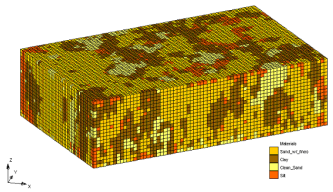
- All data set values are calculated at every node in the mesh.

SEEP2D Commands

Menu Command	Description
New Simulation...	
Delete BC	
Delete Simulation...	
Check Simulation...	
Run SEEP2D...	
Read Solution...	
Analysis Options...	
Display Options...	
Node BC...	
Flux BC...	
Export to Levee Analyst DB...	

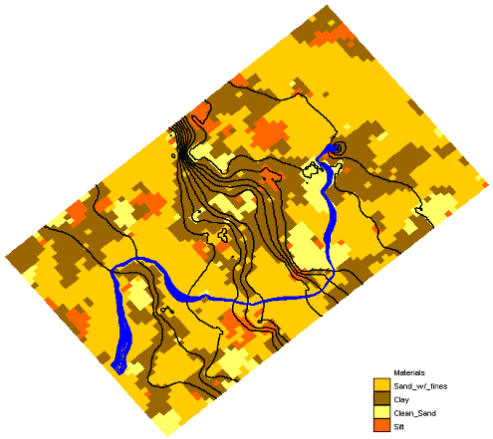
6.12. T-PROGS

T-PROGS

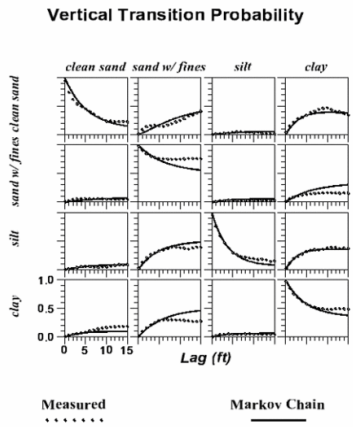
T-PROGS	
 *T-PROGS Screenshot*	
Model Info	
Model type	transition probability geostatistics on borehole data
Developer	Steven Carle
Documentation	T-Progs Manual [1]
Tutorials	T-PROGS Tutorials

GMS includes an interface to the T-PROGS software developed by Steven Carle. The T-PROGS software is used to perform transition probability geostatistics on borehole data. The output of the T-PROGS software is a set of N material sets on a 3D grid. Each of the material sets is conditioned to the borehole data and the materials proportions and transitions between the boreholes follows the trends observed in the borehole data. These material sets can be used for stochastic simulations with MODFLOW. A sample material set generated by the TPROGS software is shown below. The T-PROGS software can also be used to generate multiple input datasets for the HUF package.

T-PROGS Interface



MODFLOW solution for a T-PROGS grid. Black lines are head contours and blue lines are pathlines for an extraction well.



Observed transition probabilities (circles) and Markov chain model (solid lines) for a set of borehole data with four materials.

The T-PROGS software utilizes a transition probability-based geostatistical approach to model spatial variability by 3-D Markov Chains, set up indicator co-kriging equations, and formulate the objective function for simulated annealing. The transition probability approach has several advantages over traditional indicator kriging methods. First, the transition probability approach considers asymmetric juxtapositional tendencies, such as fining-upwards sequences. Second, the transition probability approach has a conceptual framework for incorporating geologic interpretations into the development of cross-correlated spatial variability. Furthermore, the transition probability approach does not exclusively rely on empirical curve fitting to develop the indicator (cross-) variogram model. This is advantageous because geologic data are typically only adequate to develop a model of spatial variability in the vertical direction. The transition probability approach provides a conceptual framework to geologic insight into a simple and compact mathematical model, the Markov chain. This is accomplished by linking fundamental observable attributes – mean lengths, material proportions, anisotropy, and juxtapositioning – with Markov chain model parameters.

The first step in using T-PROGS is to import a set of borehole data. The borehole data are then passed to a utility within T-PROGS called GAMEAS that computes a set of transition probability curves as a function of lag distance for each category for a given sampling interval. A sample set of measured transition probability curves are shown by the dashed lines in the following figure.

Each curve represents the transition probability from material j to material k. The transition probability $t_{jk}(h)$ is defined by:

$$t_{jk}(\mathbf{h}) = \Pr\{k \text{ occurs at } \mathbf{x}+\mathbf{h} \mid j \text{ occurs at } \mathbf{x}\}$$

[2]

where x is a spatial location, h is the lag (separation vector), and j,k denote materials. Note that the curves on the diagonal represent auto-transition probabilities, and the curves on the off-diagonal represent cross-transition probabilities.

The next step in the analysis is to develop a Markov Chain model for the vertical direction that fits the observed vertical transition probability data. The Markov Chain curves are shown as solid lines in the preceeding figure. Mathematically, a Markov chain model applied to one-dimensional categorical data in a direction Φ assumes a matrix exponential form:

$$\mathbf{T}(h_\phi) = \exp(\mathbf{R}_\phi h_\phi)$$

[3]

where h denotes a lag in the direction Φ, and RΦ denotes a transition rate matrix

$$R_\phi = \begin{bmatrix} r_{11,\phi} & \cdots & r_{1k,\phi} \\ \vdots & \ddots & \vdots \\ r_{k1,\phi} & \cdots & r_{kk,\phi} \end{bmatrix}$$

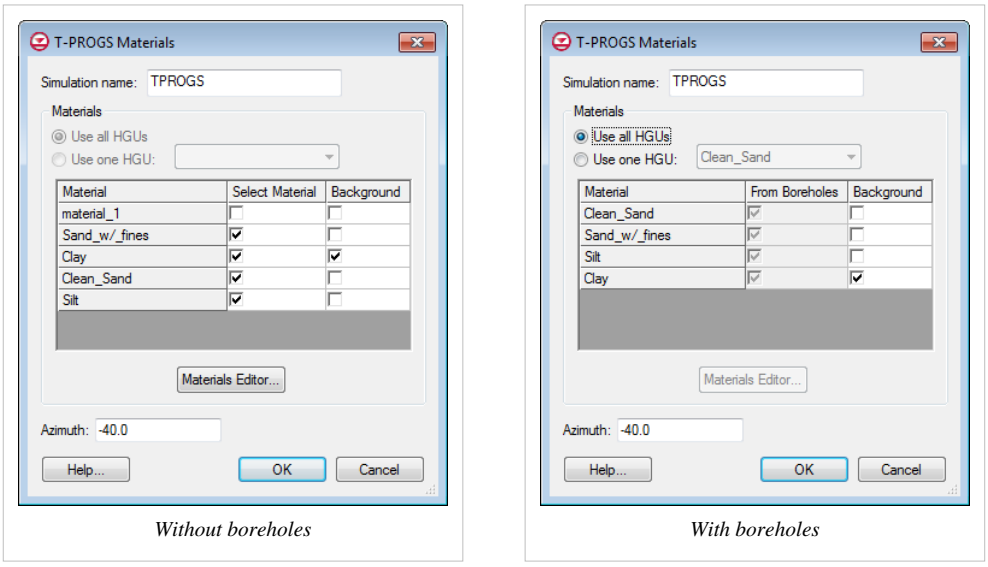
with entries r_{jk},f representing the rate of change from category j to category k (conditional to the presence of j) per unit length in the direction Φ. The transition rates are adjusted to ensure a good fit between the Markov Chain model and the observed transition probability data.

Once the Markov chain is developed for the z direction from the borehole data, a model of spatial variability must be developed for the x and y directions. Borehole data are typically not sufficiently dense in these directions. However, the x and y-direction Markov chains can be developed by assuming that the juxtapositional tendencies and the proportions observed in the vertical direction also hold true in the horizontal directions. The modeler then provides an estimate of the ratio of the mean lengths in the x and y directions relative to the z direction, and the transition rate matrices for the x and y directions can be formulated. The x, y, and z Markov chains are converted into a continuous 3D Markov chain using the MCMOD utility within T-PROGS.

In the final phase of setting up a transition probability analysis using T-PROGS, the modeler creates a grid, specifies the number of model instances (N), and launches the TSIM utility. The TSIM code uses the 3D Markov chain to formulate both indicator cokriging equations and an objective function for simulated annealing. It generates stochastic simulations using a combination of modified versions of the GSLIB codes SISIM and ANNEAL.

T-PROGS Materials

T-PROGS Materials dialog with and without borehole data.



Without boreholes *With boreholes*

When a user selects the ***New Simulation*** command to initialize a T-PROGS simulation, the *T-PROGS Boreholes* dialog appears. Here the user can select to use all boreholes or only the boreholes in a particular folder.

Boreholes use materials to define both soils and HGUs. HGUs can be used to group several materials into one hydrogeologic unit. The *T-PROGS Materials* dialog lets the user choose to use the materials in all HGUs or those from just one HGU. This feature can be used to limit the portion of the boreholes that are used in the T-PROGS simulation.

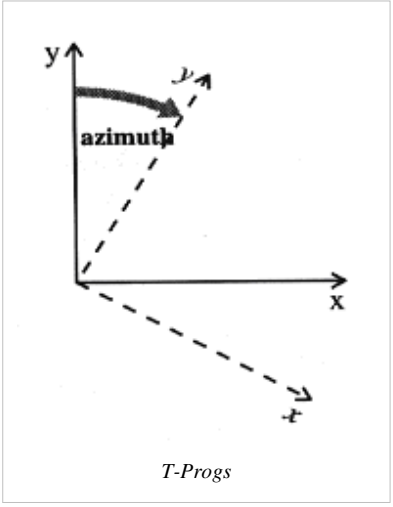
If boreholes do not exist in the model, an unconditioned simulation will be generated. In this case, in the *T-PROGS Materials* dialog the user selects the materials to be used and a corresponding background material. The upper part of the dialog lists the materials in the boreholes. The first column of toggles indicates which materials are to be used in the analysis. By default, all materials associated with the boreholes are selected. These toggles are necessary since it is possible that there may be materials defined in the materials list that are not associated with boreholes. The second column in the top section of the dialog lists the background material. By default, the material type that had the predominant occurrence in the boreholes (greatest proportion) is marked as the background material. When defining the transition probability data in the next section, the input parameters do not need to be edited for the background material. The parameters for this material are automatically adjusted to balance the equations.

Background Material

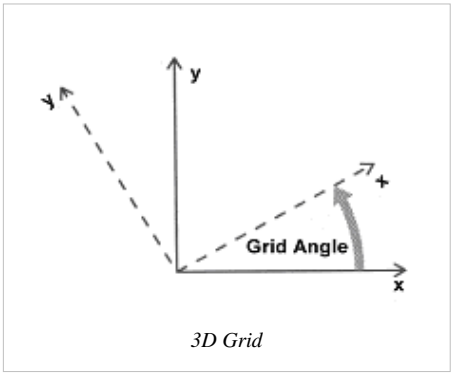
Application of the transition probability approach involves the designation of a background material. The probabilistic constraints of the Markov chains make it unnecessary to quantify data for one category. Not only is it unnecessary, but it is futile to do so because values will be overwritten in order to satisfy constraints. Conceptually, the background material can be described as the material that "fills" in the remaining areas not occupied by other units. For example, in a fluvial depositional system, a floodplain unit would tend to occupy area not filled with higher-energy depositional units and would therefore be a logical choice for the background material.

Azimuth

Azimuths for T-PROGS and 3D Grid.



T-Progs



3D Grid

The user also enters an azimuth in this dialog. The azimuth determines the orientation of the primary directions of the depositional trends in the strike/dip directions. These trends generally are aligned with the primary directions of horizontal flow in the aquifer. Theoretically, the azimuth can be oriented independently from the grid orientation. However, in practice, if the grid and azimuth orientations are offset by more than about 40^{o}, checkerboard patterns appear in the indicator array results. Hence, the azimuth orientation is set equal to the grid orientation by default. However, the grid angle is defined counterclockwise, and the azimuth angle is clockwise. Therefore, if the grid angle is 40^{o}, then the azimuth angle will be -40^{o} by default. If there is anisotropy in the xy plane, the azimuth angle should be set to the principle direction of the anisotropy. If anisotropy is not present, this angle should be coincident with the x-axis (the rows or j-direction) of the grid.

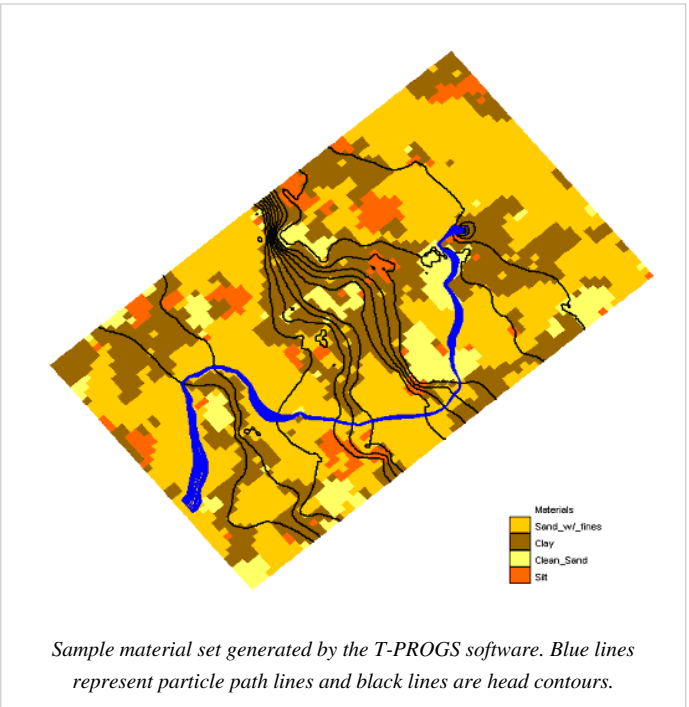
Material Limit

One limitation for both the cases with and without boreholes is that a maximum of five materials can be used in the T-PROGS algorithm. This limitation was imposed to keep the data processing and user-interface reasonably simple. Although five materials present a limitation, borehole data can generally be easily condensed down to five or fewer materials. Furthermore since this is a stochastic approach, which is based on probability, the detail generated with numerous materials is rarely justifiable anyway. In addition, as the number of materials increase, the ratio of process time to detail becomes inefficient.

Generating Material Sets with T-PROGS

The underlying equations solved by the T-PROGS software require an orthogonal grid with constant cell dimensions (X, Y, and Z). The delta X values can be different from the delta Y and delta Z values, and the delta Y values can be different from the delta Z values, but all cells must have the same change in X, Y, and Z dimensions. The MODFLOW model is capable of using the Layer Property Flow (LPF) Package with the Material ID option for assigning aquifer properties. With this option, each cell in the grid is assigned a material id and the aquifer properties (Kh, Kv, etc.) associated with each material are automatically assigned to the layer data arrays for the LPF package when the MODFLOW files are saved. The T-PROGS software generates multiple material sets (arrays of material ids), each of which represents a different realization of the aquifer heterogeneity. When running a MODFLOW simulation in stochastic mode, GMS automatically loads each of the N material sets generated by the T-PROGS software and saves N different sets of MODFLOW input files. The N solutions resulting from these simulations can be read into GMS and used to perform risk analyses such as probabilistic capture zone delineation.

One-Layer MODFLOW Grids



Sample material set generated by the T-PROGS software. Blue lines represent particle path lines and black lines are head contours.

Although MODFLOW is a three-dimensional model, a majority of the MODFLOW models constructed by typical users are 2D models consisting of one model layer. There are several reasons why 2D models are so common. One reason is that many of these models are regional models where the aquifer thickness is very small compared to the lateral extent of the model. As a result, the flow directions are primarily horizontal and little improvement is gained by adding multiple layers to the model. Even with local scale models, the aquifer thickness is often small enough that one-layer models are considered adequate. 2D models are also attractive due to the simplicity of the model increased computational efficiency. One of the problems associated with using multiple layers for MODFLOW models with unconfined aquifers is that as the water table fluctuates, the upper cells may go dry. These cells will not rewet even if the water table subsequently rises, unless the rewetting option has been selected in the flow package (BCF, LPF, or HUF). The rewetting issues can often be avoided with a one-layer model.

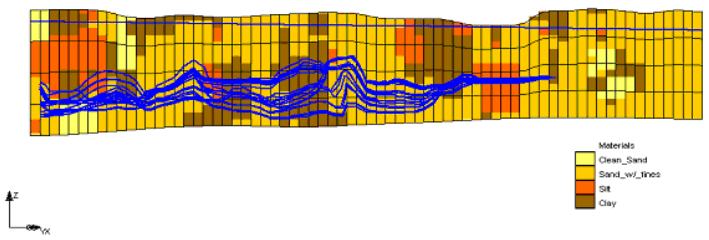
When developing a one-layer model, the modeler must determine how to distribute the hydraulic conductivity values within the layer. One option is to assume a homogenous aquifer; this is typically a gross over-simplification since aquifers are usually highly heterogeneous. Therefore, a common approach is to delineate zones of hydraulic

conductivity by examining the subsurface stratigraphic data. In many cases, these data are in the form of borehole logs. These borehole logs often exhibit substantial heterogeneity and don't always exhibit definitive trends between adjacent boreholes. Furthermore, the boreholes are often clustered with large regions of the model lacking any borehole data. The modeler then faces a difficult task of trying to determine a rational approach to delineating two-dimensional zones of hydraulic conductivity based on complex 3D borehole data.

As part of this research, we developed a technique for developing 2D zones of hydraulic conductivity from borehole logs using transition probability geostatistics. The technique is simple, fast, and preserves proportions and trends exhibited by the borehole data. The algorithm parses through each borehole and computes a predominant material at each borehole. When T-PROGS runs, the predominant material for each borehole is assigned to its corresponding location in the one-layer grid, and during the quenching process, simulations are conditioned to those data points.

Generating HUF Data with T-PROGS

Using transition probability geostatistics with MODFLOW models results in two basic limitations. First, the underlying stochastic algorithms used by the T-PROGS software are formulated such that the MODFLOW grid must have uniform row, column, and layer widths. The row width can be different from the column width, but each row must have the same width. This results in a uniform orthogonal grid. While MODFLOW grids are orthogonal in x and y, the layer thickness is allowed to vary on a cell-by-cell basis. This makes it possible for the layer boundaries to accurately model the ground surface and the tops and bottoms of aquifer units. If a purely orthogonal grid is used, irregular internal and external layer boundaries must be simulated in a stair-step fashion either by varying material properties or by activating/inactivating cells via the IBOUND array. A second limitation is that in order to get a high level of detail in the simulated heterogeneity, the grid cell dimensions are generally kept quite small. This can result in difficulties in the vertical dimension. The large number of layers with small layer thicknesses near the top of the model generally ensures that many of the cells in this region will be at or above the computed water table elevation (for simulations involving unconfined aquifers). As a result, these cells will undergo many of the numerical instabilities and increased computational effort issues associated with cell wetting and drying.



Sample HUF stratigraphy data generated by the T-PROGS software. Blue lines represent particle path lines and water table.

The Hydrogeologic Unit Flow (HUF) package released with MODFLOW 2000 makes it possible to overcome both of these limitations resulting in a powerful mechanism for incorporating transition probability geostatistics in MODFLOW simulations. With the HUF package, the modeler is allowed to input the vertical component of the stratigraphy in a grid-independent fashion. The stratigraphy data are defined using a set of elevation and thickness arrays. The first array defines the top elevation of the model. The remaining arrays define the thicknesses of a series of hydrogeologic units, starting at the top and progressing to the bottom of the model. For each array of thicknesses, many of the entries in the array may be zero. This makes it possible to simulate complex heterogeneity, including pinchouts and embedded lenses that would be difficult to simulate with the LPF and BCF packages.

The T-PROGS interface in GMS includes an option for integrating transition probability geostatistics results with the HUF package. The basic approach used by the option is to overlay a dense background grid on the MODFLOW grid and run T-PROGS on the background grid. A set of HUF arrays is then extracted from the background grid for use with the MODFLOW model. To use this option, user should first create a MODFLOW grid with the desired number of layers and the layer elevations should be interpolated to match the aquifer boundaries. The row and column widths are uniform but the layer thicknesses may vary from cell to cell. Then, when TSIM is launched, the HUF option

should be selected. GMS then generates a background grid that encompasses the MODFLOW grid. The rows and columns of this grid match the MODFLOW grid but the layer thicknesses are uniform and relatively thin, resulting in a much greater number of layers than the MODFLOW grid. The user specifies the number of layers in this background grid. A T-PROGS simulation is then performed to get a set of material sets on the background grid. Each of the material sets in the T-PROGS output is then transferred from the background grid to a set of HUF elevation/thickness arrays. The HUF top elevation array is set equal to the top of the MODFLOW grid. The thickness arrays are then found by searching through the background grid to find the bottom elevations of contiguous groups of indicators. The elevations from these groups are then added to an appropriate elevation array in the HUF input. The resulting set of HUF input arrays are listed in GMS Project Explorer. By clicking on each item in the Project Explorer, the selected set of HUF arrays are loaded into the HUF package and the corresponding stratigraphy is displayed in the GMS window. The multiple HUF input arrays can be used to perform a stochastic simulation.

Notes

[1] http://gmsdocs.aquaveo.com/t-progs.pdf

Vertical Markov Chain

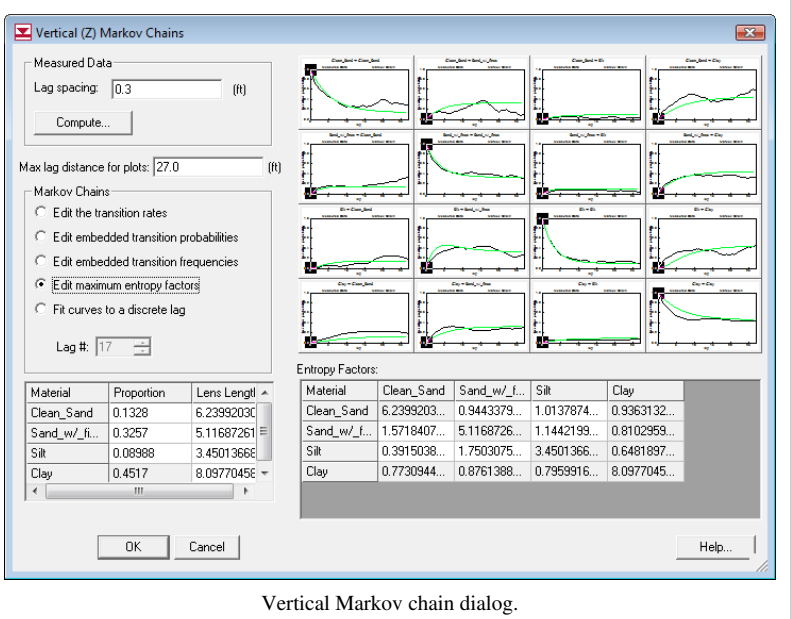
A dialog assists the user in defining the vertical Markov chains. This dialog is composed of three main sections:

- Plot section
- Markov Chains section
- Spreadsheet section

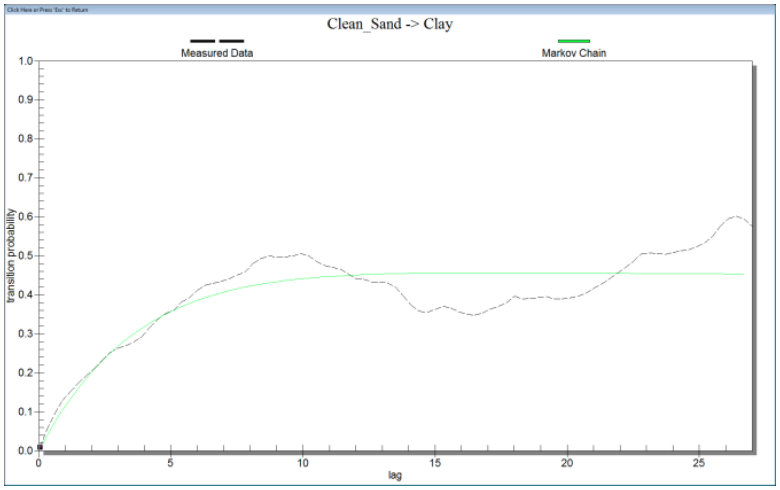
All three sections enable the user to develop a 1-D Markov chain in the vertical direction.

Plot section

The plot section includes the array of curves, the Lag spacing edit field, the Compute button, and the Max lag distance for plots edit field. The number of plots in the array produced correlates to the number of materials used in the simulation. If N materials are used, an N by N array of plots will illustrate the transition probabilities for each material with respect to every other material. Every plot is labeled with a name and units and can be maximized with a command in the menu produced by right-clicking on the curve in question. The curves are automatically regenerated anytime a change is made in the other sections of the dialog.



Vertical Markov chain dialog.



Transition probability plot.

Each of the plots contains two curves depicting the transition probability. The dashed line represents the transition probability measured from the borehole data by the GAMEAS utility. In general, this curve represents the transition probability from material j to material k. The transition probability $t_{jk}(h)$ is defined by:

$$t_{jk}(\mathbf{h}) = \Pr\{k \text{ occurs at } \mathbf{x}+\mathbf{h} \mid j \text{ occurs at } \mathbf{x}\}$$

[1]

where x is a spatial location, h is the lag (separation vector), and j,k denote materials. The lag is defined by the Lag spacing item in the upper left corner of the *Vertical (Z) Markov Chains* dialog. The curve shown with the solid line is called a “Markov Chain”. The Markov Chains are used to formulate the equations used by T-PROGS to generate the multiple material sets during the simulation stage. The objective of this stage of the analysis is to fit the Markov Chain curves as accurately as possible to the measured transition probability curves. This process is similar to fitting a model variogram to an experimental variogram in a kriging exercise. The transition rates are adjusted to ensure a good fit between the Markov Chain model and the observed transition probability data.

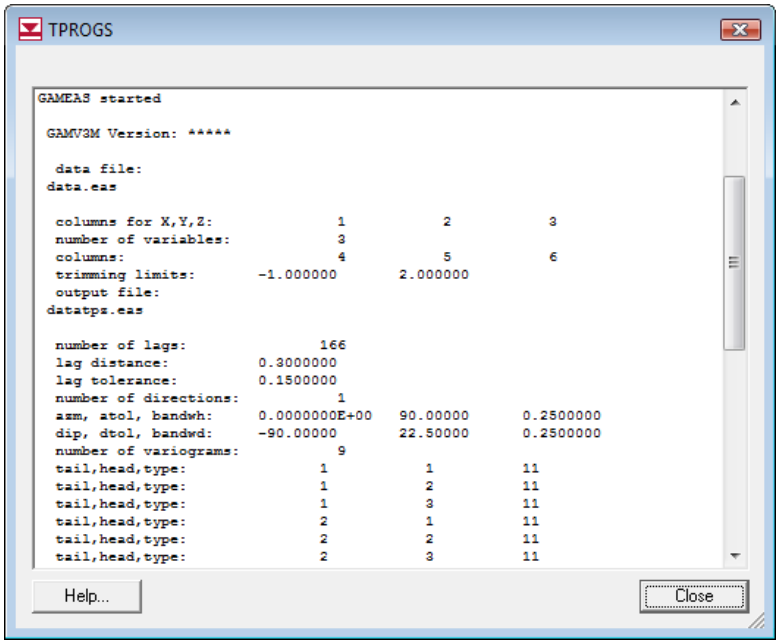
It should be noted that the self-transitional curves on the diagonal start at a probability of 1.0 and decrease with distance and the off-diagonal curves start at zero probability and increase with distance. In both cases, the curves eventually flatten out at some distance. The probability corresponding to the flat part of the curve represents the mean proportion of the material. All curves on a particular column should flatten out to the same proportion. The proportions are displayed in the lower left corner of the dialog. The point where a tangent line from the early part of the curves on the diagonal intersects the horizontal (lag distance) axis on each curve represents the mean lens length for the material. The mean lens lengths are shown just to the right of the mean proportions in the lower left part of the dialog. The slope at the beginning of each of the Markov Chains represents the transition rate. Together, the proportions, lens lengths, and transition rates define the Markov Chains.

Several methods are provided for fitting the Markov Chains to the measured transition probability curves. These methods are listed in the section of the dialog titled *Markov Chains*. By default, GMS automatically makes an attempt to fit the curves using the **Edit maximum entropy factors** option. In many cases, this fit is sufficiently accurate and we can proceed to the next step. However, it is often useful to explore the other options for fitting the curves.

If boreholes exist in the model, the **Compute...** button becomes undimmed. When the user clicks the **Compute...** button, the parameter files required for running GAMEAS are generated and GAMEAS is executed.

GAMEAS

GAMEAS is an algorithm that processes borehole data and determines geologic characteristics such as material proportions and transition probability curves in a given direction. A separate window displays the details of the GAMEAS run, which allows the user to monitor the output from the GAMEAS simulation.



GAMEAS executable inside GMS interface.

When GAMEAS completes a successful run, the results, including the material proportions and transition probability curves from the measured data, are read into the corresponding data fields in the *Vertical Markov Chain* dialog. Furthermore, the transition rates which correspond to the slope of the transition probability curves when the lag equals 0 are interpolated from the measured data curves. In addition to running GAMEAS, the code parses through the borehole data and calculates the embedded transition probabilities and frequencies. These values are stored in arrays that correspond to options #2 and #3 in the Markov Chains section of the dialog.

Lag

The Lag spacing determines how dense the curves are, and the Max lag distance for plots determines the range of the curves. The curves always range from 0 to the Max lag distance for plots horizontally, and they range from 0 to 1 vertically to honor probability constraints.

Markov chains section

There are five alternate methods of generating Markov chains in this section (area in the *Vertical Markov Chain* dialog). These methods are in a radio-button configuration to allow the user to conveniently change from one method to another. Each of these five methods will be described.

- Edit the transition rates
- Edit embedded transition probabilities
- Edit embedded transition frequencies
- Edit maximum entropy factors
- Fit curves to a discrete lag
- Edit the transition rates

Edit the transition rates

With this option one can directly edit the array of transition rates that are listed in the Transition Rates section. This option is useful after selecting the Compute button and running GAMEAS because slopes can be inferred from the measured data curves. GAMEAS outputs transition probability curves. Transition rates used in this option correspond to the slope of the transition probability curve at a lag = 0. When reading the output from GAMEAS, the transition probability rates are interpolated as

$$r_{jk,\phi} = 0.57 * r1_{jk,\phi} + 0.29 * r2_{jk,\phi} + 0.14 * r3_{jk,\phi}$$

where r1, r2, and r3 are the slopes defined by a straight line from the origin out to lag1, lag2, and lag3 respectively. As the lag approaches zero, more weight should be given to the corresponding slope. Hence, a weight of 0.57, 0.29, and 0.14 were assigned to r1, r2, and r3 respectively. Once the slopes are computed for each entry in the matrix, the mean lengths for each category are computed by

$$\bar{L}_{j,\phi} = \frac{-1}{r_{jj,\phi}}$$

Regardless of which Markov Chain option is selected, the background row and column, Sand_w/_fines, is dimmed because the values in this row and column are automatically computed from the remaining entries by probability constraints of the background material. In addition, with this option selected, the Lens Length column is also dimmed because the lens lengths are automatically computed and updated from the diagonal terms in the Transition Rates spreadsheet. The diagonal terms of the Transition Rates spreadsheet must be negative to obey probability rules. With this data, this method produces an accurate fit between the measured (green) and the Markov chain (blue) curves at small lag spaces.

Edit the embedded transition probabilities

This is a more intuitive method of generating Markov chains and is conducive to sites with and without data. It is conducive to sites with data because the embedded transition probabilities can be determined from the borehole data. When a simulation is initialized, if borehole data exist default embedded transition probabilities are computed from the borehole data. If borehole data do not exist, the embedded transition probabilities can be estimated with some basic geologic knowledge including the average mean lengths of each material for each direction and depositional trends.

With this option selected, the diagonal terms are dimmed because these values are derived from the values entered in the Lens Length column. Adjusting the proportions, lens lengths, or the off-diagonal terms in the Transition Rates spreadsheet alters the curves.

With this option, the spreadsheet in the lower right of the dialog represents the probability that the row material will transition to the column material moving vertically upwards in the +Z direction.

Edit the embedded transition frequencies

This option is similar to option #2, except embedded transition frequencies populate the off-diagonal terms of the Transition Rates spreadsheet. Embedded transition frequencies are also computed from borehole data when a simulation is initialized if borehole data exist. Once again, this is an intuitive framework with geologic knowledge including average mean lengths and depositional trends.

Edit maximum entropy factors

While this option can be used with borehole data, it is ideally suited for cases without borehole data. With this option, the user edits the proportions for all but the background material and the mean lens lengths for all materials. The lens lengths are used to populate the diagonal terms of the Transition Rates spreadsheet, and the maximum entropy factors fill the off-diagonal terms of the spreadsheet. The maximum entropy factors represent the ratio of the transition rate to the maximum entropy transition rate. A maximum entropy factor of 1.0 represents maximum disorder in depositional tendencies. A rate greater than 1.0 indicates that the two categories tend to occur next to each other. A factor less than unity would infer the opposite. This is an intuitive method of generating Markov chains and is conducive to all types of sites. This method enables logical incorporation of anisotropy into the model with the maximum entropy factors.

Fit curves to a discrete lag

This option is only undimmed if a transition probability curve from measured data exists in memory. When this option is selected, the **Lag #** edit field is undimmed and the user enters the discrete lag the curves will be fit to.

This option produces Markov chains that are computed from the measured transition rates produced by GAMEAS. GAMEAS computes a set of transition probabilities at each lag specified by the user. This option computes an array of transition rates from the slope of the curves generated by GAMEAS (green). The transition rates correlate to the shape of the curve from the origin to the lag # specified by the user in the Lag # edit field. Therefore, the cells of all the spreadsheets in the dialog are dimmed because the values are inherited from the measured curves (green). The values in the spreadsheets change depending on the lag # entered. By adjusting the lag interval, an excellent fit can often be obtained.

Spreadsheet section

This section includes two separate spreadsheets: Transition Rates and Proportions & Mean Lengths spreadsheets. The Transition Rates spreadsheet contains the rate entries that correspond to the selected option in the Markov Chains section. The Proportions column holds the proportions for each material. The Mean Lengths column contains the average mean length in the vertical direction for each material. The data in these spreadsheets define the Markov chains.

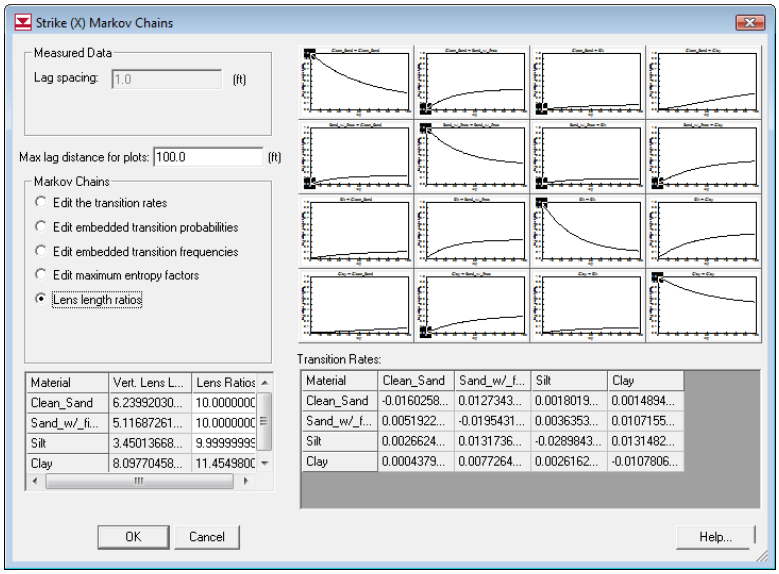
Notes

Strike Dip Markov Chain

Once the vertical Markov chains have been defined, the user is then presented with the *Strike (X) Markov Chains* dialog. This dialog has the same general setup as the vertical dialog.

Strike (X) Markov Chains

There are three minor differences between this dialog and the vertical dialog. The first difference is in the Markov Chains section. The option, Lens width ratios, replaces the Fit curves to a discrete lag option. The Fit curves to a discrete lag option is not applicable because horizontal measured transition probability curves do not exist due to lack of data in the horizontal direction. The Lens width ratios option is the default option and should be used in most cases. This option allows users to apply the transition data entered in the vertical direction to the horizontal direction. The proportion data are directly inherited from the vertical data.



Strike/Dip Markov chain dialog.

The second change is in the Spreadsheet Section. Rather than entering the mean lengths, the user enters a ratio corresponding to the ratio of the lens length in the x direction to the lens length in the z direction. For example, if the lens length for material A is 5 feet in the z direction and the user enters 10.0 for the ratio, then the lens length in the x direction would be 50 feet. The Lens Width Ratios option is particularly useful because the only required input is lens length ratios for the non-background materials. The remaining data are all inherited from the vertical data. The third change is in the Plot Section. Due to the lack of measured data in the horizontal direction, each plot contains only one curve: the Markov chain curve.

Vertical→Lateral Data Conversion

Typical site stratigraphic data is conducive to developing vertical spatial variability. However, rarely is the quantity of data adequate to develop an accurate model in the lateral directions. The combination of Walther's Law and the transition probability approach allows for a logical method of developing lateral spatial variability from vertical spatial variability. Walther's Law states that vertical successions of deposited facies represent the lateral succession of environments of deposition. Therefore, a logical method of generating a 3-D model of spatial variability would be first to develop a 1-D Markov chain in the vertical direction based on site data, assuming there is such data. Second, using Walther's Law and geologic knowledge, one can develop lateral, strike and dip, Markov chains of spatial variability. However, one issue that arises when applying vertical transition trends to lateral directions is how to cope with asymmetric vertical trends like fining upwards. For example, if in the vertical direction, sand tends to deposit on gravel as would be typical in a fluvial deposition, there will be a transition rate associated with the transition of "sand→gravel" and "gravel→sand". The transition of "gravel->sand" will be greater than "sand→gravel" because of the fining upward trend. However, in the lateral direction, which of these transition rates should be applied? Although the trend of sand next to gravel remains in the lateral direction, the transition rates of "sand→gravel" and "gravel→sand" should be equivalent or symmetric as defined by

$$r_{jk} = \frac{p_k}{p_j} r_{kj}$$

The strategy for averaging the vertical transition rates to come up with the lateral rates is given in the three steps below.

1. Compute the lower-half rate (R-ls) that will satisfy symmetry with the upper-half rate (R-u) for the vertical data using the symmetry relation.
2. Set the lower-half rate for the lateral direction (R'-l) equal to (R-l + R-ls)/2
3. Compute the upper-half rate for the lateral direction (R'-u) that will satisfy symmetry with the new lower-half rate (R'-l) using the symmetry relation.

In addition to the averaging technique applied to the off-diagonal terms of the lateral transition rates, an adjustment was made to the diagonal terms of the rate matrix. It will be remembered that the diagonal terms correlate to the average mean lengths by

$$\bar{L}_{j,\phi} = \frac{-1}{r_{jj,\phi}}$$

Generally, in depositional patterns, lateral mean lengths are larger than their counterparts. Therefore, the lateral mean lengths generally need to be increased by a factor F prescribed by the user. This factor F is equal to the ratio of the lateral mean lengths/vertical mean lengths. If the mean length for category K increases by a factor F, the corresponding transition rate will decrease by that same factor F. And the row sum for category K must therefore decrease by the factor F.

Dip (Y) Markov Chains

The dip dialog has an identical appearance and functionality as the strike dialog.

TSIM

When a T-PROGS simulation has been created, TSIM can be run to generate either material sets on a 3D grid or HUF data for MODFLOW. TSIM is run via the ***TPROGS|Run TSIM*** menu command. This brings up the TSIM Wizard.

Step 1

You can choose to run TSIM now from GMS or save the input files so you can run TSIM later. If you don't run TSIM from GMS, no material sets or HUF arrays will be created.

Step 2

Running TSIM from GMS

Option	Description
Number of realizations	The number of material sets or HUF sets that will be generated.
Seed	The random number seed used by TSIM. This is generated by GMS but can be changed by the user. Running TSIM with the same inputs and see will result in identical outputs.
Max. # of quenching iterations	A TSIM parameter. "No more than five quenching iterations are usually necessary – too many iterations may produce unrealistic artifacts."[1]
Quenching tolerance	A TSIM parameter. "The tolerance limit sets a criteria for terminating quenching based on the value of the objective function as normalized relative to its initial value."
TSIM Output	You can choose to generate material sets or, if a MODFLOW model exists which uses the HUF package, HUF arrays.
Create material probability datasets	This will cause datasets to get created, one per material, where the dataset values equal the probability that that material occurs in the given cell.
Background Grid	The dimensions and number of grid ranks of the background grid are determined from the 3D grid in the project. If generating HUF arrays you can specify the number of grid layers in the vertical (Z) direction.
Target grid layers	Starting at GMS version 8.0 you can target a subset of grid layers. The resulting material sets will have inactive values outside of the targeted area. You can specify the min and max layers or the named layer ranges you wish to target.

Saving files to run TSIM later

The option in Step 2 if saving the TSIM files for later use are similar to those for running TSIM in GMS. You must specify a file and where it is to be saved. Also, the dimensions and number of ranks of the background grid must be specified. Finally, no material sets or HUF arrays will be generated.

Notes

T-PROGS Commands

Menu Command	Description
New Simulation...	
Delete Simulation	
Materials...	
Vertical (Z) Markov Chains...	
Strike (X) Markov Chains...	
Dip (Y) Markov Chains...	

6.13. TOUGH

TOUGH

TOUGH	
Model Info	
Model type	Transport Of Unsaturated Groundwater and Heat
Developer	Lawrence Berkeley National Laboratory
Documentation	TOUGH Documentation [1]

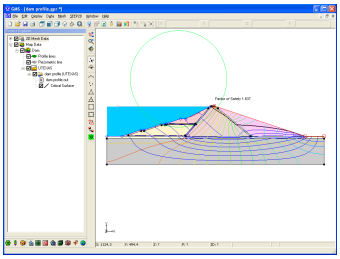
Some individuals have worked to allow GMS to be used as a pre- and post-processor for TOUGH [2] (Transport Of Unsaturated Groundwater and Heat), a numerical model maintained by the Lawrence Berkeley National Laboratory [3]. More information is available here [1]. Also, see this paper [4] and this paper [5].

References

[1] http://esd.lbl.gov/research/projects/tough/software/processors.html
[2] http://esd.lbl.gov/research/projects/tough/
[3] http://www.lbl.gov/
[4] http://www.sciencedirect.com/science/article/pii/S0098300410003742
[5] http://esd.lbl.gov/FILES/research/projects/tough/events/symposia/toughsymposium12/Borgia_Andrea-Venezia.pdf

6.14. UTEXAS

UTEXAS

UTEXAS	
 *UTEXAS Screenshot*	
Model Info	
Model type	Slope stability
Supported versions	4.1.0.3
Developer	Dr. Stephen G. Wright
Documentation	UTEXAS Manual [1] UTEXAS Addendum [2] TexGraph4 Manual [3]
Tutorials	UTEXAS Tutorials

UTEXAS is a slope stability software package created by Dr. Stephen G. Wright of the University of Texas at Austin. UTEXAS is used to analyze slope stability using the limit equilibrium method. The user provides the geometry and shear strength parameters for the slope in question and UTEXAS4 computes a factor of safety against slope failure. The factor of safety for a candidate failure surface is computed as the forces driving failure along the surface divided by the shear resistance of the soils along the surface. UTEXAS4 is a state-of-the-art slope stability code and has been widely used in industry for many years.

GMS versions 6.5 and later include an interface to UTEXAS which allows users to create UTEXAS input files using GMS.

Creating a Model

Existing UTEXAS models can be imported into GMS, or new models can be created from scratch. The UTEXAS interface is entirely within the map module. The model consists of a conceptual model and one or more coverages.

- Importing

  To import an existing UTEXAS model, use the standard ***File|Open*** command. The file to import is the UTEXAS input file. This file may have a *.dat extension which is (unfortunately) the extension UTEXAS expects. GMS creates the UTEXAS conceptual model and coverages from the file being imported.

  Aspects of UTEXAS models can also be imported from a GeoStudio file.

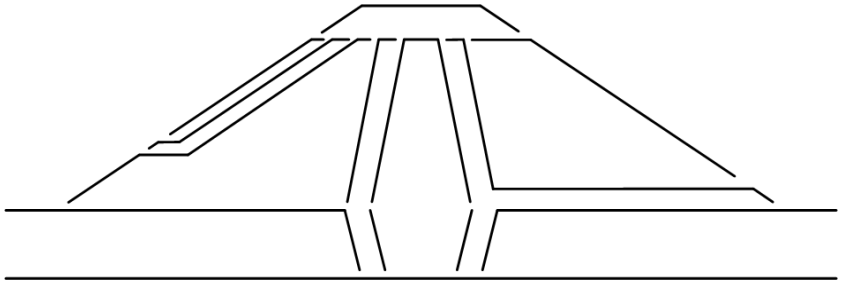
- Creating in GMS

  Creating a UTEXAS model in GMS can be done a variety of ways. The UTEXAS tutorials illustrate these methods.

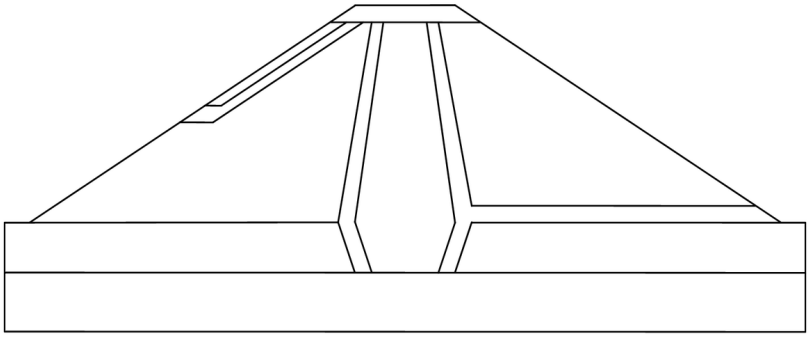
  - Type in the feature point coordinates, then connect the points with arcs

- Create feature arcs with the mouse
- Convert a CAD drawing to feature objects

Profile Lines vs. Arcs and Polygons



Profile lines depicting a dam. Gaps show where lines begin and end (no gaps would exist in an actual model).



Polygons depicting a dam

Profile Lines

UTEXAS uses "profile lines" to define the soil stratigraphy. A profile line is a series of connected points that must go from left to right (or bottom to top) and represent the top of a soil layer. The profile line does not close on itself, and does not cross any other profile lines.

Polygons

GMS does not use profile lines, but instead uses arcs and polygons to define the soil stratigraphy. Using polygons is much easier than using profile lines because there is no need to worry about how to break up the lines such that they all go from left to right (or bottom to top).

When GMS saves the UTEXAS input file, it automatically figures out the profile lines that UTEXAS needs to represent the soil stratigraphy. When importing a UTEXAS file, GMS automatically builds arcs and polygons from the profile lines.

One notable difference between the profile line and polygon approaches is that when using polygons, the bottom-most polygon must be extended downward some distance below the bottom-most profile line to represent the bottom-most soil area.

Material Properties

UTEXAS soil material properties are entered in GMS using GMS materials. Each feature polygon has a material associated with it.

Pore Water Pressure

There are various ways to define pore water pressure. Two of the methods are more advanced: the piezometric line method, and the interpolated pressure method.

Piezometric Line

UTEXAS allows the pore water pressure to be specified using a piezometric line. In GMS, a piezometric line is an arc that is in it's own feature coverage (since the arc will likely overlap arcs in the profile line coverage). The material that uses the piezometric line can specify the coverage the piezometric line (arc) is in.

Interpolated Pressure

Another method for specifying the pore water pressure is "Pressure Interpolated" which uses a set of points where each point has a value representing the pore pressure at that point. In GMS, you can do this by associating a data set from a 2D mesh with the material. The dataset might come from a SEEP2D solution, since SEEP2D is a model in GMS that can solve for pore pressures.

Integration with SEEP2D

SEEP2D is a 2D seepage analysis model that, when combined with UTEXAS, provides a complete and a powerful 2D profile analysis solution. Since these two models are closely related, the conceptual model type for UTEXAS is called "SEEP2D/UTEXAS". One could use the same conceptual model to create both a SEEP2D model and a UTEXAS model. The UTEXAS tutorials illustrate this.

Running UTEXAS

UTEXAS model icon as it appears in the Project Explorer

UTEXAS differs from most models supported by GMS in the way that it is run. Most model codes supported by GMS can be run from inside GMS. Since UTEXAS is a Windows application with no command line options (yet), this is not possible.

Also, GMS typically provides a model wrapper for most of the supported models as a convenient way to watch the progress of the model and automatically read in the results upon completion. Again, since UTEXAS is a Windows application, it is not possible to use a model wrapper.

To run UTEXAS:

- Export the model from GMS
- Launch UTEXAS (outside of GMS)
- Open the exported file in UTEXAS
- Wait for UTEXAS to finish
- Read the solution into GMS

Exporting the Model

To save a UTEXAS model that is in GMS in preparation for running UTEXAS, right-click on the UTEXAS model icon under the conceptual model and select the ***Export*** command. Note that GMS uses the extension *.utx instead of *.dat when saving the UTEXAS input file.

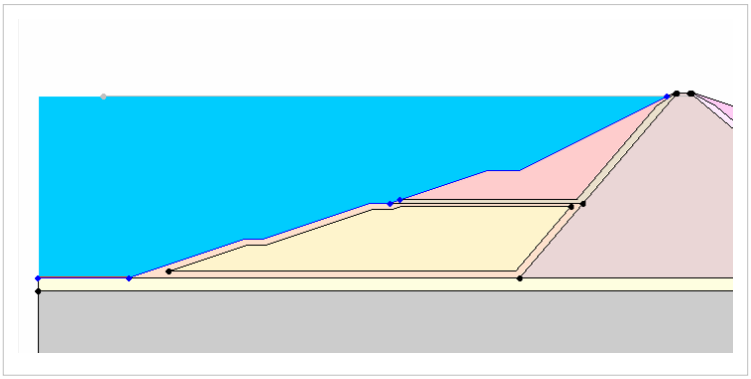
Reading the Solution

To read the solution generated by UTEXAS into GMS, right-click on the UTEXAS model icon under the conceptual model and select the ***Read Solution*** command. The UTEXAS solution will have an extension of *.out.

Display Options

A number of display options are associated with UTEXAS. To find these, select the **Display Options** button, click on the *Map Data* item from the list, and select the *UTEXAS* tab on the right.

UTEXAS Display Options

Option	Description
Distributed loads	Arcs that are designated as distributed loads. Arrows are drawn at the spacing and scale specified to show the loading.
Head	 Arcs designated as Head arcs have the space above them filled with the specified color.
Starting circle	The starting circle specified in the *UTEXAS Analysis Options* dialog.
Factor of safety	If a solution exists, the factor of safety.
Critical surface	If a solution exists, the critical surface.
Limiting depth	The limiting depth specified in the *UTEXAS Analysis Options* dialog.
Tangent line	The horizontal tangent line specified in the *UTEXAS Analysis Options* dialog.

Unsupported Features

Not all of the features of UTEXAS are currently supported in the GMS interface. Support for more features will be added in future versions of GMS. The following features are not supported.

Command Words

- LABel
- NO compute
- OTHer units
- SIUnits /or/ SI
- UT3
- UT4
- '***'

Group B, Profile Lines

- Table 6.2, Group B - Profile Line Data Input Format - Import Mode

Group C, Material Properties

- Table 7.1, Group C - Material Property Data Input Format
  - Line 4
    - Reference (R)
    - Anisotropic shear (A)
    - Interpolate Strengths (I S) (version 7.0 and earlier. Supported starting at GMS version 7.1)
  - Line 6
    - Interpolate Ru values (I R)

Group D, Piezometric Line

- Table 8.1, Group D - Piezometric Line Data Input Format
  - Line 2
    - Field 2, Unit weight of water

Group E, Interpolation Data

- Table 9.1 - GMS will export this table but cannot import it
- Table 9.2 - GMS won't import or export this table

Group G, Distributed Loads

- Table 11.1, Group G - Distributed Load Data Input Format for Individual Points
  - Line 2
    - Field 4, Shear stress

Group K, Analysis/Computation

- Table 14.2a
  - Line 3
    - Field 1, "T" (or "TANGENT") (version 7.0 and earlier. Supported starting at GMS version 7.1)
- Table 14.2c, "Fixed" Grid
  - Line 3
    - Field 1, "T" (or "TANGENT") (version 7.0 and earlier. Supported starting at GMS version 7.1)
- Table 14.2d, "Fixed" Grid
  - Not supported in version 7.0 and earlier. Supported starting at GMS version 7.1. Also, although multiple criteria can be used to specify the radius, GMS only supports using one.
- Table 14.3, Summary of Sub-Command Words for Group K Data
  - 1 (Same as "SIN" which GMS does support)
  - 2 (Same as "TWO" which GMS does support)
  - 3 (Same as "THR" which GMS does support)
  - ARC (Arc length)
  - BAS (Base length)
  - CHA (Change)
  - CRI (Critical shear surface)
  - FAC (Factor of Safety)
  - FOR (Force imbalance)
  - INC (Increments for subdivision)
  - ITE (Iteration)
  - MIN (Minimum weight)
  - MOM (Moment imbalance)
  - PAS (Passes)
  - RES (Restrictions)
  - SAV (Save "n" most)
  - SEI (Seismic coefficient) (version 7.0 and earlier. Supported starting at GMS version 7.1)
  - SID (Side force inclination)
  - SOR (Sort radii)
  - STO (Stop)
  - SUB (Subtended angle)
  - TRI (Trial)
  - UNI (Unit weight of water)
  - UNS (Unsort)
- %206.5/models/UTEXAS4%20Manual.pdf UTEXAS4 Manual [4]
- %206.5/models/UTEXAS4%20Addendum.pdf UTEXAS4 Addendum [4]
- Dr. Stephen G. Wright [5]
- UTEXAS article on Wikipedia [6]

- Jun 1987 CETN-III-34 Checking Stability of Bulkheads Located in Ports, Harbors and Coastal Waterways Against Shear Failure Computer Program: UTEXAS2 [7]

References

[1] http://gmsdocs.aquaveo.com/UTEXAS4%20Manual.pdf
[2] http://gmsdocs.aquaveo.com/UTEXAS4%20Addendum4.pdf
[3] http://gmsdocs.aquaveo.com/TexGraf4%20Manual.pdf
[4] ftp://pubftp.ems-i.com/download/GMS/GMS
[5] http://www.ce.utexas.edu/prof/wright/home.html
[6] http://en.wikipedia.org/wiki/UTEXAS
[7] http://chl.erdc.usace.army.mil/library/publications/chetn/pdf/cetn-iii-34.pdf

UTEXAS Display Options

The properties of all UTEXAS properties that GMS displays on the screen can be controlled through the UTEXAS tab of the *Display Options* dialog. This dialog is opened by right clicking on the Map Data entry in the Project Explorer, selecting the ***Display Options*** command, and then selecting the UTEXAS tab. This tab is only visible when there is a UTEXAS simulation. It can also be accessed from the from the *Display* menu or the **Display Options** macro. The following table describes the display options available for the UTEXAS model.

Display Option	Description
Distributed loads	Controls the display of arrows representing distributed loads placed on an embankment or dam. The line color can be adjusted by clicking on the button to the right of the toggle. If the **Auto X spacing** is toggled on, the arrows will automatically be distributed along the length of the distributed load. However, the user can specify the X spacing by turning off and the **Auto X spacing** toggle and specifying an X spacing the edit field. This value represents a real world value. The **Auto Y scale** controls the length of the arrow tails representing the distributed load. If the **Auto Y spacing** toggle is turned off, the arrow tails will be drawn using the Y scale specified in the edit field.
Head	Controls the display of the head fill color. The head will be displayed as filled polygon representing the amount of head that is acting on an embankment. This color can be adjusted by clicking on the button to the right of the toggle.
Starting circle	Controls the display of the line representing the starting circle to be used by UTEXAS in performing the slope stability analysis. The line type, line width, and line color can be changed by clicking the on button to the right of the toggle.
Factor of safety	Controls the display of the factor of safety computed by the UTEXAS simulation. The font type, font size, and font color can be adjusted by clicking the on button to the right of the toggle.
Critical surface	Controls the display of the line representing the critical surface determined by the UTEXAS simulation. The line type, line width, and line color can be adjusted by clicking the on button to the right of the toggle.
Limiting depth	Controls the display of the line representing the limiting depth to be used in the UTEXAS simulation. The line type, line width, and line color can be changed by clicking the on button to the right of the toggle.

UTEXAS Commands

Menu Command	Description
Analysis Options...	
Export...	
Launch UTEXAS4...	
Read Solution...	
Export to Levee Analyst DB...	

6.15. WASH123D

WASH123D Display Options

The properties of all WASH123D boundary conditions that GMS displays on the screen can be controlled through the WASH123D tab of the *Display Options* dialog. This dialog is opened by right clicking on the 3D Mesh Data entry in the Project Explorer, selecting the ***Display Options*** command, and then selecting the WASH123D tab. This tab is only visible when there is a FEMWATER simulation. It can also be accessed from the from the *Display* menu or the **Display Options** macro. The following table describes the display options available for the WASH123D model.

Display Option	Description
Well	Controls the display of well flow boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Well (super pump node)	Controls the display of well super pump nodes flow boundary conditions. The fill color can be adjusted using the button to the left of the display toggle. The radius of the well can also be adjusted in the edit field below the Well (super pump node) toggle.
Head	Controls the display of head flow boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Equivalent head	Controls the display of equivalent head flow boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Spec. flux	Controls the display of specified flux flow boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Variable flux	Controls the display of variable flux flow boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Enforced total head	Controls the display of enforced total head flow boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Init. enforced total head	Controls the display of initial enforced total head flow boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Discharge x-sect.	Controls the display of discharge cross section flow boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Flux	Controls the display of flux boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Well conc.	Controls the display of well concentration transport boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Spec. conc.	Controls the display of specified concentration transport boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Spec. mass flux	Controls the display of specified mass flux transport boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
Variable conc.	Controls the display of variable concentration transport boundary conditions. The symbol, symbol size, and symbol color can be adjusted using the button to the left of the display toggle.
BC values	Controls the display of boundary condition values. The font, font size, and font color can be adjusted using the button to the left of the display toggle.
Display symbol legend	Controls the display of a legend containing the symbols for the boundary conditions used in the FEMWATER simulation.

Check All	By clicking this button, all of the display options are turned on.
Check None	By clicking this button, all of the display options are turned off.

7. Modeling

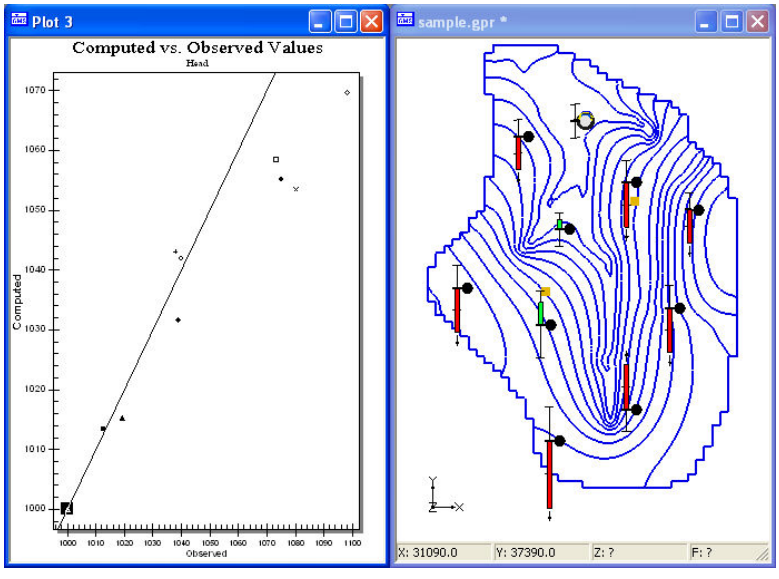
7.1. Calibration

Model Calibration

Calibration is the process of modifying the input parameters to a groundwater model until the output from the model matches an observed set of data. GMS includes a suite of tools to assist in the process of calibrating a groundwater model. Both point and flux observations are supported. When a computed solution is imported to GMS, the point and flux residual errors are plotted on a set of calibration targets and a variety of plots can be generated showing overall calibration statistics. Most of the calibration tools can be used with any of the models in GMS. Automated Parameter Estimation is supported for MODFLOW models via PEST.

Two types of observations can be defined in GMS: point observations and flow observations. Both types of observations are defined in the map module and are associated with points, arcs, and polygons. Point observations represent locations in the field where some value has been observed. In most cases, the points will correspond to observation wells and the value will be the elevation of the groundwater table (the head). Flow observations represent linear or areal objects such as streams and reservoirs where the gain or loss between the aquifer and the object has been measured or estimated. Both point and flow observations can be assigned a confidence interval or calibration target. While point observations can be used with any model, flow observations can only be used with MODFLOW.

Once a set of observed point and flow values has been entered, each time a model solution is imported, GMS automatically interpolates the computed solution to the observation points. For some models (MODFLOW) the model outputs the computed values at the observation points. Also, MODFLOW outputs the computed flow for the flow observations. A calibration target representing the magnitude of the residual error is displayed next to each observation point and each flow object as shown below. The size of the target is based on the confidence interval or the standard deviation. In addition to the calibration targets next to the observation points, you can choose to display any of a number of statistical plots.



Calibration Targets and Plots of Calibration Statistics.

Automated Parameter Estimation

One of the tools provided in GMS for model calibration is automated parameter estimation. With automated parameter estimation, an external utility, sometimes called an "inverse model", is used to iteratively adjust a set of parameters and repeatedly launch the model until the computed output matches field-observed values. Parameter estimation is used in conjunction with the point observations and the flow observations.

Automated parameter estimation is supported in GMS for the MODFLOW simulations using PEST a general purpose parameter estimation utility developed by John Doherty of Watermark Computing.

Inverse models should only be used carefully and with a full understanding of the assumptions, equations, and methods involved. It is suggested that the user read the available documentation on the inverse model being used. Only the steps involved in setting up an inverse model are described in this document.

Basic Steps

The basic steps involved in using an inverse model for parameter estimation are follows:

1. Create a Working MODFLOW Model

The first step is to create your MODFLOW model and run a simulation. Before launching the inverse model, you need to have a MODFLOW model that successfully converges and you need to determine a good set of starting values for your parameters. Once you have a solution it is also a good idea to copy the computed heads from your solution to your starting heads array. This ensures that as the inverse model modifies the parameters and runs MODFLOW repeatedly, it is more likely that MODFLOW will quickly converge each time it is launched.

2. Enter the Observations

Once you have a working MODFLOW model, you should enter your head and flux observations. Head observations are entered as points using an observation coverage in the Map module. Flow observations are assigned directly to arcs and polygons in source/sink coverages. Each of the observations is assigned a weight that is saved to the inverse input files.

3. Turn on the Inverse Model

You must select an inverse model. Bring up the Global Options dialog and select either the Parameter Estimation or Stochastic Inverse Model button depending on whether a stochastic simulation is being run.

4. Parameterize the model

The next step is to parameterize your model. See the Parameters page for more details.

5. Create a Parameter List

The next step is to create the parameter list. See the Parameters page for details.

6. Set parameter estimation options

Once the parameter list is set up, you may wish to edit the general Parameter Estimation options. These options include the output control and convergence criteria.

7. Edit the Group Weight Multipliers

The group weight multipliers can be edited to adjust the relative weight of the head and flux observations.

8. Edit the PEST ASP Package

Edit the MODFLOW PEST ASP Package if necessary in order to ensure a stable solution.

9. Save and Run MODFLOW Model

Once all of the inverse model options have been set, the next step is to save the MODFLOW model using the ***Save/Save As*** command in the *File* menu. Next, run MODFLOW and the inverse model will run with MODFLOW. The inverse model will then be launched in a separate window or the model wrapper in which you will see information relating to the MODFLOW runs and the status of the objective function. Depending on the problem, the inverse model may take anywhere from several minutes to several hours (or days) to run to completion. When the inverse process is completed successfully, GMS automatically launches a MODFLOW forward run with the optimal values computed by the inverse model. Thus, the solution will reflect the optimal values computed by the inverse model.

10. Viewing the Optimal values

When the inverse model is finished, it writes out a text file containing the set of parameter values corresponding to the minimum calibration error. These values can be viewed with the Import Optimal Values button. This copies the optimal parameter values to the Starting Value field in the Parameter List.

Sensitivity Analysis

At each PEST iteration, PEST computes the sensitivities of each of the parameters. This information is available in the "*model*.sen" file (where *model* is the name of the MODFLOW model). PEST records the composite sensitivity and the relative composite sensitivity of each parameter in this file. This information is useful in determining which parameters have the greatest effect on the model as well as which parameters have the least effect on the model. Thus, the "insensitive" parameters can be removed or held constant in a subsequent PEST run.

For a more detailed description of parameter sensitivity see section 5.3.2 of the PEST manual.

Parameter Estimation Dialog

Options affecting parameter estimation can be changed via the Parameter Estimation Dialog.

Parameter Estimation Dialog

The Parameter Estimation dialog allows the editing of inverse modeling options that are specific to PEST. This dialog is available when Parameter Estimation is chosen as the Run option in the *Global Options\Basic Package* dialog.

Max number of iterations (NOPTMAX)

This value (NOPTMAX) sets the maximum number of optimisation iterations that PEST is permitted to undertake on a particular parameter estimation run. If you want to ensure that PEST termination is triggered by other criteria, more indicative of parameter convergence to an optimal set or of the futility of further processing, you should set this variable very high. A value of 20 to 30 is often appropriate.

If NOPTMAX is set to 0, PEST 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 particular parameter set and/or to inspect observation residuals corresponding to that parameter set.

If NOPTMAX is set to −1, PEST 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 supplied in the PEST control file.

Max number of iterations with no improvement (NPHINORED)

If PEST has failed to lower the objective function over NPHINORED successive iteration it will terminate execution. A value of 3 or 4 is often suitable for this variable.

Advanced Options

Max number of relative convergence iterations (NPHISTP); Relative convergence limit (PHIREDSTP)

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

$(\Phi i - \Phi min)/\Phi i \leq PHIREDSTP$ (4.6)

(Φi being the objective function value at the end of the i'th optimisation iteration and Φmin being the lowest objective function achieved to date), PEST will consider that the optimisation process is at an end.

For many cases 4 and 0.01 are suitable values for NPHISTP and PHIREDSTP respectively. However you must be careful not to set NPHISTP too low if the optimal values for some parameters are near or at their upper or lower bounds. In this case it is possible that the magnitude of the parameter upgrade vector may be curtailed over one or a number of optimisation iterations to ensure that no parameter value overshoots its bound. The result may be smaller reductions in the objective function than would otherwise occur.

Max number of relative parameter change iterations (NRELPAR); Relative parameter change criterion (RELPARSTP)

If the magnitude of the maximum relative parameter change between optimisation iterations is less than the Relative Parameter Change Criterion (RELPARSTP) over Max # of Relative Parameter Change Iterations (NRELPAR) successive iterations, PEST will cease execution.

All adjustable parameters, whether they are relative-limited or factor-limited, are involved in the calculation of the maximum relative parameter change. RELPARSTP is a real variable for which a value of 0.01 is often suitable. NRELPAR is an integer variable; a value of 2 or 3 is normally satisfactory.

Max relative parameter change per iteration This (RELPARMAX) is the maximum relative change that a parameter is allowed to undergo between optimisation iterations.

Max factor parameter change per iteration (FACPARMAX)

This value is the maximum factor change that a parameter is allowed to undergo during an iteration.

Run-time matrix options

Select these options if you want these arrays written to external files. These arrays will also be written to the PEST output file (*.rec).

Measurement obj func upper limit (PHIMLIM)

This 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 minimise the regularisation objective function Φr.

Measurement obj func accept. level (PHIMACCEPT)

This is the acceptable level for the measurement objective function that PEST uses to change its method of calculating the Marquardt Lamdas (see PEST documentation).

Normally PHIMACCEPT should be about 5% to 10% greater than PHIMLIM. However if PEST is performing well, you may wish to make it closer to PHIMLIM than this. In choosing the best parameter set at any stage of the optimisation process (for recording in the parameter value file) PEST looks at all parameter sets for which it has carried out model runs up to that point in the process. If any of these runs have resulted in an objective function less than PHIMACCEPT, it then searches from among these runs for the parameter set which gave rise to the lowest regularisation objective function. If PHIMACCEPT is set too close to PHIMLIM, PEST's selection of the best parameter set may be restricted somewhat, for there may be some parameter sets for which the measurement objective function Φm is just above PHIMACCEPT but for which Φr is quite low. Alternatively, if PHIMACCEPT is set too large, then PEST might not try hard enough to reduce Φm to Φmi, preferring instead to work within the weaker constraint set by PHIMACCEPT. When working in regularisation mode, PEST prints out Φr and Φm for every parameter upgrade attempt. It will be apparent from this information whether PHIMACCEPT has been set correctly.

FRACPHIM

PEST ignores the value supplied for FRACPHIM unless it is greater than zero. A value of between zero and 1.0 (but normally less than about 0.3) can be supplied for this variable if you are unsure what value to use for PHIMLIM. See the PEST documentation.

Automatic user intervention (AUI)

When the optimization process undertaken by PEST appears to be going nowhere, the situation can often be remedied by selectively withdrawing certain parameters (normally the most insensitive ones) from the parameter estimation process. This process has been automated in PEST using the AUI option. For more information on AUI see the PEST documentation (section 5.7 of the PEST manual).

It should be noted that use of the SVD process in PEST is usually more effective than AUI as the SVD process removes insensitive parameters.

Parallel PEST

GMS allows you to run PEST in parallel on a single machine to take advantage of multiple cores. This can greatly speed up the PEST runs.

- Number of slaves

  "Slaves" refers to the separate processes that will be run in parallel. You can specify the number of slaves or, if not specified, GMS will automatically determine the number of cores available on the machine and use that for the number of slaves.
- Wait time

  The wait time is the amount of time that PEST will pause at certain strategic places in their communication. Normally the default value should work fine. However, if either PEST reports a sharing violation on your hard drive then you should increase the value of the wait time.

SVD (Singular Value Decomposition)

The *Use SVD* toggle is available to turn on the SVD functionality in PEST. For a more complete explanation of SVD, see the PEST manual [1] in section 8.4. The inputs to the SVD process can be edited by selecting the **SVD Options** button.

The SVD process analyzes the parameters that are currently part of the parameter estimation process and removes parameters that are not helping to solve the problem. The user can limit the number of parameters used by specifying a maximum number of singular values (MAXSING) or by specifying EIGTHRESH. By default MAXSING is set to 1000 and EIGTRESH to 1E-7, so that the number of parameters will be limited by the value of EIGTHRESH.

- MAXSING – maximum number of singular values to include in the inversion process.
- EIGTHRESH – a ratio of the lowest to highest parameter eigen value (a value of 1E-7 is usually sufficient).
- EIGWRITE – controls output written to the *.svd file by PEST. When the value is 1 a more verbose file is written that can become quite large. By default the value of EIGWRITE is set to 0.

SVD-Assist

The **Use SVD-Assist** toggle turns on the SVD-Assist process for PEST. This process is particularly advantageous for models that have hundreds or thousands of parameters (such as pilot points). SVD-Assist involves 3 basic steps.

1. First, PEST runs MODFLOW once for every parameter in order to compute a matrix. This information is used to create super parameters that are combinations of the parameters originally specified.
2. Second, SVDAPREP is run to create a new PEST control file. The options for SVDAPREP are entered by selecting the **SVD-Assist Options** button. For more information on each of these options see the PEST manual in section 8.5.4.2. The most important option entered is the *Specify # super param* and this is set to **No** by default. When this option is set to No, then the information written to the *.svd file will be used to specify the number of super parameters.
3. Third, PEST runs using the new control file written by SVDAPREP. This should result in significantly fewer model runs for each PEST iteration. This often results in an order of magnitude reduction in the number of runs required for each PEST iteration.

Tikhonov Regularization

Tikhonov Regularization (prior information for pilot points). This section of the dialog allows the user to select the method for include Tikhonov regularization in the PEST run. If neither option is turned on then regularization will not be included in the PEST run.

The first option, Preferred homogeneous regularization, is the option that GMS has always supported with pilot points. When using this option, prior information equations are included that impose a homogeneity constraint on the pilot points. This means that in absence of other information, pilot points that are near to one another should have about the same value.

- Prior information power factor

  This is used to change the weight applied to the prior information equations for the pilot points. A value of 1 is normally sufficient. The prior information equations impose a homogeneity constraint on the pilot points. This means that in absence of other information, pilot points that are near to one another should have about the same value. When the prior information equations are created GMS will compute an inverse distance weight between each pilot point and all other pilot points for a given parameter. This weight is then raised to the power of the *Prior information power factor* and assigned to the equation for a given pair of points. So to increase the homogeneity constraint (assign a higher weight to the prior information equation), the user should decrease this value. To decrease the homogeneity constraint (assign a lower weight to the prior information equation), the user should increase this value.

The second option, Preferred value regularization, is a new option beginning with GMS version 8.0. When this option is used, prior information equations are included that constrain the pilot points near their starting values. Using this option the user can give a set of starting values to the pilot points based on field data or professional judgment. PEST will only change those values if necessary to calibrate the model.

Also new in GMS 8.0, parameters of different types (HK, RCH) are put into different regularization groups. According to John Doherty, this helps differentiate weighting amongst pertinent prior information equations.

References

[1] http://gmsdocs.aquaveo.com/pest.pdf

PEST

PEST is a general purpose parameter estimation utility developed by John Doherty of Watermark Computing. The PEST interface in GMS can be used to perform automated parameter estimation for MODFLOW. The steps involved in setting up a PEST run are described in the automated parameter estimation topic.

The PEST options are edited by selecting the ***Parameter Estimation*** command in the *MODFLOW* menu and then clicking on the PEST tab.

PEST version support

The following table shows the version of PEST supported by different versions of GMS. To see the latest released version of PEST visit http://www.pesthomepage.org/Downloads.php.

GMS	PEST
GMS 6.5	PEST 10.0
GMS 7.0	PEST 10.0
GMS 7.1	PEST 12.0
GMS 8.0, 8.1, 8.2	PEST 12.1
GMS 8.3, 9.0	PEST 12.2
GMS 9.1	PEST 12.3

Run Options

Once the MODFLOW simulation has been initialized, the next step is to enter the data required by the Global Options/Basic package. This includes data defining fundamental program options such as the computational time intervals (stress periods), an array defining which cells are inactive and which cells have constant heads, an array of starting head values for a transient simulation, and a set of flags defining which of the other packages are to be used. The input data for this package should be entered before editing any of the other packages. The MODFLOW *Global Options\Basic Package* dialog is accessed through the ***Global Options*** command in the *MODFLOW* menu. The options in the dialog are as follows:

Headings

The two headings are optional text strings which are written to the MODFLOW text output file.

Version

The MODFLOW version can be specified with the choices being (as of July 2013):

- MODFLOW-2000
- MODFLOW-2005
- MODFLOW-NWT

The following choices will soon be added to the list:

- MODFLOW-LGR
- MODFLOW-USG

Additionally, the type of binary executable can be specified using one or more of the following choices:

- Double precision
- Parallel
- 64 bit

Run Options

The run options are not part of the actual MODFLOW input files, but present different ways that MODFLOW 2000 can be run from GMS.

Forward Run

A forward run is a normal MODFLOW simulation. If parameters have been defined for either a stochastic or parameter estimation run, the mean or starting values of the parameters are used for the forward run.

Sensitivity Analysis

The sensitivity analysis option is used to perform a sensitivity analysis on a set of selected parameters. The results can be presented with a set of plots or by contouring data sets representing grid sensitivities. This option is only available with the LPF and HUF flow packages. This option is not available in GMS 6.5 and later (see MODFLOW with HDF5).

After running PEST, sensitivities are displayed in the .sen file. Click here for more information.

Parameter Estimation

In the parameter estimation mode, a set of parameters is found that minimizes the residual between observed and simulated heads and flows. These options are described in more detail on the Automated Parameter Estimation page. This option is only available with the LPF and HUF flow packages.

Stochastic Simulation

The stochastic simulation option is used to perform a stochastic simulation using the Monte Carlo or Latin Hypercube methods for randomizing a selected set of parameters. Stochastic simulations can also be performed using a material set approach (indicator simulations). A risk analysis wizard can be used to analyze the results for a probabilistic threshold analysis or a probabilistic capture zone delineation. These options are described in more detail on the stochastic simulation page.

Stochastic Inverse Model

If the material set option is used for stochastic simulations, the "stochastic inverse" option can be used to perform automated parameter estimation on each of the N candidate model instances in the stochastic. The weighted RMS errors for each of the resulting optimized solutions can be used to weight the computations performed by the risk analysis wizard. This option is only available with the LPF and HUF flow packages.

Model Type

The simulation can be designated as either steady state or transient. If a steady state simulation is specified, certain portions of the MODFLOW interface such as the *Stress Period* dialog are inactivated since they are not relevant.

No Flow Head

This is the value of head to be assigned to all inactive (no flow) cells (IBOUND=0) throughout the simulation.

Stress Periods

The Stress Periods button is used to bring up the *Stress Period* dialog. The stress periods should be defined before any of the sources/sinks are entered. If the steady state option is selected, the **Stress Periods** button is dimmed.

Packages

The Packages button brings up the *Packages* dialog.

Units

The Units button the *Basic Package* dialog brings up the *Units* dialog.

IBOUND

Values

The IBOUND button of the *Global Options\Basic Package* dialog brings up the array editor. The IBOUND array contains a value for each cell in the grid defining the type of the cell as constant head, inactive, or variable head.

Constant Head

A negative value indicates that the cell has a constant head. The value of the constant head is defined in the starting heads array.

Inactive

An IBOUND value of zero indicates that the cell is inactive (no-flow).

Variable Head

A positive IBOUND value indicates that the cell has a variable head (i.e., the head value will be computed as part of the simulation).

Editing the IBOUND Array

There are several ways to change the active/inactive status (positive vs. zero) of a cell before or after initializing the IBOUND array. One method is to directly edit the IBOUND array using the *IBOUND* dialog. Another method is to select the ***Cell Attributes*** command in the *MODFLOW* menu. In most cases, the most efficient method is to use the ***Activate Cells in Coverage*** command in the Map module. This method uses a polygon to define the active and inactive regions.

The constant head cells are typically assigned or edited in one of three ways. One method is to directly edit the IBOUND array. Another method is to select a set of cells and use the *Cell Properties* dialog in the *MODFLOW* menu. The simplest method is to define the constant head zones using feature objects as part of a conceptual model in the Map module.

Starting Heads

The starting head values are used as initial conditions for head for both steady state and transient simulations. The **Starting Heads** button on the left side of the *Basic Package* dialog is used to enter the values of the starting heads array. Selecting the **Starting Heads** button brings up the MODFLOW Array Editor.

Top Elevation

The Top Elevation button brings up an array editor that allows you to edit the top elevation of each layer. GMS requires that the top and bottom elevations for adjacent layers be the same. This means that when you edit the bottom of one layer, move down to the next layer, and edit the top of that layer, the bottom of the previous layer will also be changed. Note that the top and bottom layer elevations must be entered regardless of the which layer data package (BCF, LPF, HUF) is chosen even though these values may not be used because of certain package options.

Bottom Elevation

The Bottom Elevation button brings up an array editor that allows you to edit the bottom elevation of each layer. Note that the top and bottom layer elevations must be entered regardless of the which layer data package (BCF, LPF, HUF) is chosen even though these values may not be used because of certain package options.

Confining Beds

The Layer Confining Beds dialog, accessed from the *Global Options/Basic Package* dialog, allows you to select which layers will have a confining bed below them. The last layer in the grid may not have a confining bed.

Confining beds are most common in older models where the user was trying to conserve memory in solving the groundwater model. In general, it is recommended that you explicitly model all of the layers in the system instead of using confining beds. This feature is supported in GMS to make it possible for users to read in older models.

In the spreadsheet, the user may turn on the confining bed option for any of the layers except the last layer in the grid.

The Confining Bed Elevations button brings up the array editor that allows the user to edit the elevation of each layer.

Observations

Point Observations

The primary type of field data used in a typical calibration exercise is point observations. Point observations represent values that are measured at some location in the field. Point observations generally correspond to water table elevations measured at observation wells. However, multiple observed values can be defined at each observation point. Observation points are managed in the Map module using the *Coverage Setup* dialog.

Flow Observations

Flow observations represent gains or losses between aquifers and streams or reservoirs. In addition to point observations, flow observations are an essential part of a calibration exercise for a flow model. If calibration is attempted using point observations only, there may be many combinations of parameters such as hydraulic conductivity and recharge that will result in the same head distribution. Adding one or more flow observations serves to "pin down" the flow quantity resulting in a set of hydraulic conductivities and recharge values that are more likely to be unique.

While the point observation tools are model independent, GMS only supports flow observations for MODFLOW and FEMWATER. With MODFLOW, observed flows are assigned to selected arcs and polygons making up the MODFLOW conceptual model in the Map module. When a MODFLOW solution is imported, the computed flows are read for the arcs and polygons and compared with observed values.

With a FEMWATER simulation, observed values cannot be assigned to objects in the FEMWATER conceptual model. However, when a FEMWATER solution is imported, the computed flows on selected model boundaries can be automatically summed. Comparison of computed vs. observed flows must then be made manually.

Observation Weights

When performing automated parameter estimation, a set of head and flow observations are defined using points, arcs, and polygons in the Map module. When entering the point and flow observations, care should be taken when entering the calibration interval and confidence values. These values are used to determine the weights assigned to each observation in the inverse model. The weight is multiplied by the residual for the observation in the objective function. The weight that is sent to the inverse model input files by GMS is computed as

$$\frac{1}{(\text{Standard Deviation})^2 * \text{Group Weight}}$$

Note that GMS will automatically convert from an interval and a confidence to a standard deviation or you can directly enter the standard deviation.

Group Weight Multipliers

In addition to the individual weight, a group weight can also be assigned. Group weights are assigned using the Group Weight section of the *Observations* dialog. This dialog is accessed by selecting the ***Observations*** command in the *MODFLOW* menu.

A group weight can be assigned to each of the following observation types:

1. **Head observations.**
2. **Constant head flow observations.**
3. **River flow observations.**
4. **General head flow observations.**
5. **Drain flow observations.**
6. **Stream flow observations.**

Options 2-6 correspond to flow observations that are defined using the Observed flow rate option.

The default value for the group weights is 1.0. The default value can be changed to give a larger influence to a particular observation type. For example, if a particular model had sixteen head observations and one flux observation corresponding to a stream gage, a better solution may be obtained by increasing the flux group weight to give more weight to the stream gage measurement.

Observations Dialog

This dialog is used to manage which coverages that contain MODFLOW observation data will be applied to the current simulation. It is also used to apply group weights. You can only access this dialog when observations have been created using the Map Module in a MODFLOW conceptual model.

Group Weights

These weights can be used to emphasize (or deemphasize) a type of observation for the simulation.

Coverages

This spreadsheet allows you to choose which observation coverages will be used in the current simulation. This can be helpful if you have observations for a site from different times, but you only want to use one of the times.

Export Trans. Obs.

Beginning with version 8.0, this button allows you to export a *.csv (comma separated values) file with transient observation data. This file can be loaded into excel to create plots of the transient observation values vs. the model computed values. An example of using this data is included in the MODFLOW- Managing Transient Data tutorial.

Confidence Interval and Standard Deviation

The interval and standard deviation are related by the following equation:

$$sd = \frac{CI}{z}$$

where sd is the standard deviation, CI is the confidence interval, and z is the the "z statistic" based on the specified confidence and the normal distribution. The user can enter an interval and confidence, and the standard deviation will be computed; or the user can enter a standard deviation and confidence, and the interval will be computed.

In practical terms entering an interval (or standard deviation) and confidence is an indication of how much error the user believes is associated with the observed value.

The standard deviation becomes important when using an inverse model. The weight assigned to each of the observations points is a function of the standard deviation. This weight is used in the objective function that the inverse model tries to minimize. An observation point with a small standard deviation will have a greater influence on the objective function than a point with a large standard deviation.

The user must enter an interval (or standard deviation) and confidence in the *Properties* Dialog. Although these values are rarely quantified the following examples may prove helpful.

If the user had the following set of head measurements for one observation well:

Date	Head
May 10, 1998	55.0
July 10, 1998	50.5
September 5, 1998	48.6
November 15, 1998	49.1
February 2, 1999	50.8
March 12, 1999	54.0
April 1, 1999	57.2

The mean of the data is 52.17 and the standard deviation is 3.25. The user could enter this standard deviation and a confidence of 95%.

Many times the user does not have this much data available. Usually the user will only have one measured value. In this case the user must use engineering judgement to estimate an interval or standard deviation. For example, if I have a single head measurement of 45.7 ft and I believe that observation to be accurate to within a 1 foot. Then I would enter 1 foot as my interval.

Plot Wizard

Plots are useful for many purposes, such as extracting data from two or three dimensional objects and model verification. Plots are created through the Plot Wizard.

Plot Wizard Steps

The Plot Wizard (***Display | Plot Wizard***) is used to create 2D plots. The plot wizard is composed of two steps described below. In addition, the types of plots that can be created are described and illustrated below.

Step 1

In the first step, the plot type is selected. The types include:

- Computed vs. Observed Data
- Computed vs. Observed Data (Weighted)
- Residual vs. Observed Data
- Residual vs. Observed Data (Weighted)
- Parameter Sensitivities
- Error vs. Simulation
- Error vs. Time Step
- Error Summary
- Time Series
- Active Data Set Time Series Plot
- S/S Flow vs. Time
- Flow Budget vs. Time
- Gage Package Value vs. Time

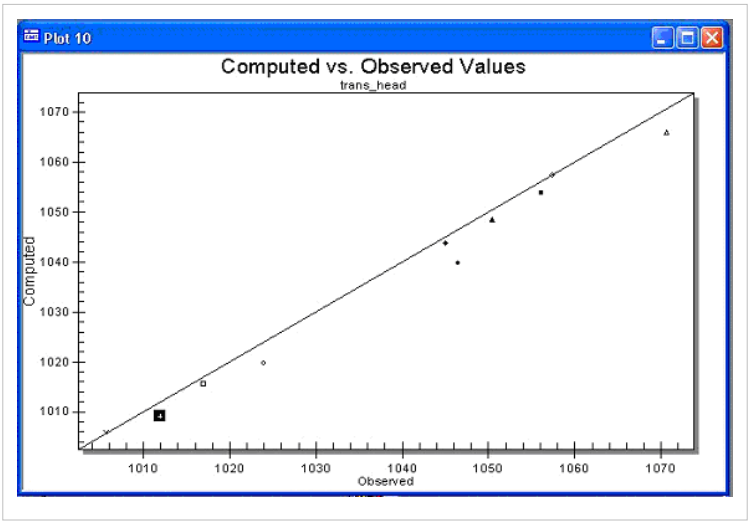
A sample and explanation are displayed for each plot type. The **Next >** button is undimmed if the necessary data for the selected plot type exists in the current project. If the **Next >** button is disabled, a help text explaining the problem is displayed below the Plot Type box.

Step 2

In the second step, the attributes of each plot are set. The attributes associated with each plot type are explained below and can be located quickly by clicking on the desired plot type listed above. The options depend on the plot type and will be described below.

Computed vs. Observed

A Computed vs. Observed plot is used to display how well the entire set of observed values match a model solution. A 45^{o} line is drawn on this plot, which represents a perfect correspondence between observed data and solution values. One symbol is drawn for each observation point at the intersection of the observed and computed values for the point. This plot can show the trend of the solution values with regard to matching the observed data. Only those points whose value is specified as observed for the selected data type will be shown in the plot. These plots are created in the Plot Wizard by setting the Plot Type to Computed vs. Observed. A sample plot is shown in the figure.



Computed vs. Observed Plot Options

The second step contains the following options.

Coverage and Measurements

The observation coverage and measurements can be selected for each plot. If only one observation coverage and measurement exist these are used by default.

Use current solution

This option causes the plot to compare the observed values with the values of the current solution and time step for each observation point. When the active solution changes, the plot is recomputed and updated. If only one solution is in memory then this option is defaulted.

Use selected solutions

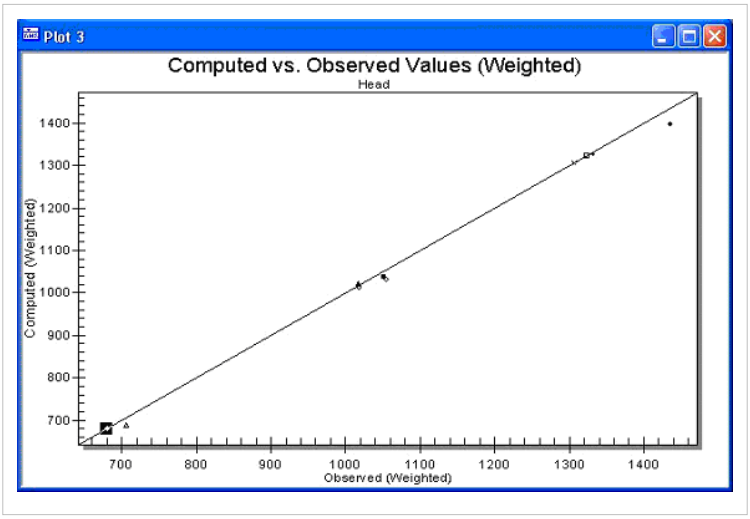
This option causes the plot to compare the observed values with the values of the specified solution for each observation point. Changing the active solution does not affect the plot.

Use time step

Because the plot shows only values from a specific time step, The Active Times Step is used by default.

Computed vs. Observed (Weighted)

A Computed vs. Observed Weighted plot is used to display how well the entire set of weighted observed values match a model solution. These weights are set by selecting the Observation item in the MODFLOW menu. A 45^{o} line is drawn on this plot, which represents a perfect correspondence between observed data and solution values. One symbol is drawn for each observation point at the intersection of the weighted observed and computed values for the point. This plot can show the trend of the solution values with regard to matching the weighted observed data. Only those points whose value is specified as observed for the selected data type will be shown in the plot. This plot is not available with transient data. These plots are created in the Plot Wizard by setting the Plot Type to Computed vs. Observed (Weighted). A sample plot is shown in the figure.



Computed vs. Observed Weighted Plot Options

After the plot type is set in the First Page of the Plot Wizard, the Next button is clicked to open the Computed vs. Observed Weighted Plot Options wizard page. This page contains the following:

Coverage and Measurements

The observation coverage and measurements can be selected for each plot. If only one observation coverage and measurement exist these are used by default.

Use current solution

This option causes the plot to compare the weighted observed values with the values of the current solution and time step for each observation point. When the active solution changes, the plot is recomputed and updated. If only one solution is in memory then this option is defaulted.

Use selected solutions

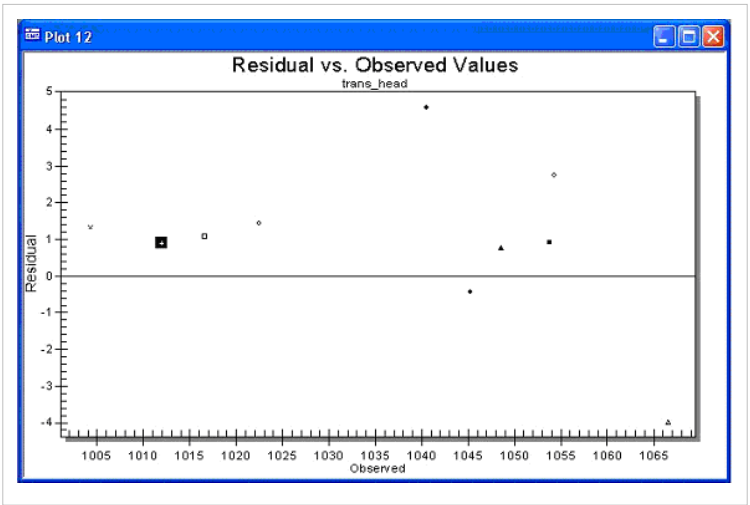
This option causes the plot to compare the weighted observed values with the values of the specified solution for each observation point. Changing the active solution does not affect the plot.

Use time step

Because the plot shows only values from a specific time step, The Active Times Step is used by default.

Residual vs. Observed

A Residual vs. Observed plot is used to display how well the entire set of observed values match a model solution. On this plot is drawn a horizontal line along an error of zero, representing what would be a perfect correspondence between observed data and solution values. Then, one symbol is drawn for each observation point at the intersection of the observed and residual (computed-observed) values for the point. This plot can show the trend of the solution values with regards to matching the observed data. Only those points whose value is specified as observed for the selected data type will be shown in the plot. These plots are created in the Plot Wizard by setting the Plot Type to Residual vs. Observed. A sample plot is shown in the figure.



Residual vs. Observed Plot Options

After the plot type is set in the First Page of the Plot Wizard, the **Next** button is clicked to open the Residual vs. Observed Plot Options wizard page. This page contains the following:

Coverage and Measurements

The observation coverage and measurements can be selected for each plot. If only one observation coverage and measurement exist these are used by default.

Use current solution

This option causes the plot to compare the observed values with the residual values of the current solution and time step for each observation point. When the active solution changes, the plot is recomputed and updated. If only one solution is in memory then this option is defaulted.

Use selected solutions

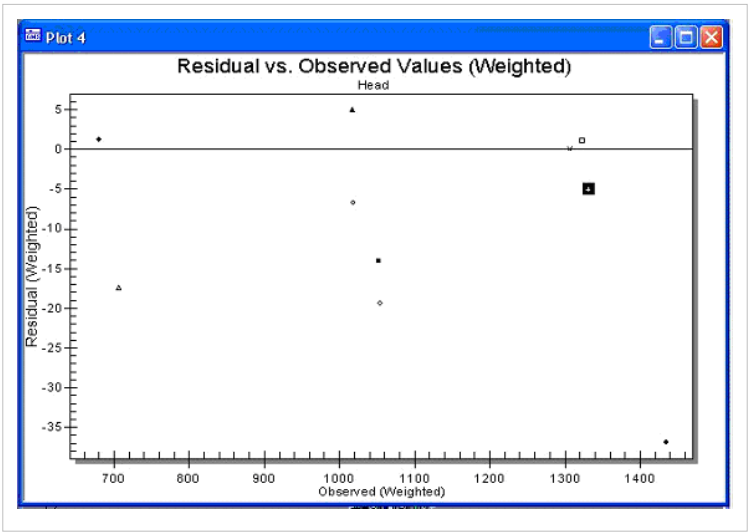
This option causes the plot to compare the observed values with the residual values of the specified solution for each observation point. Changing the active solution does not affect the plot.

Use time step

Because the plot shows only values from a specific time step, The Active Times Step is used by default.

Residual vs. Observed (Weighted)

A Residual vs. Observed (Weighted) plot is used to display how well the entire set of weighted observed values match a model solution. On this plot is drawn a horizontal line along an error of zero, representing what would be a perfect correspondence between weighted observed data and solution values. One symbol is drawn for each observation point at the intersection of the weighted observed and residual (computed-observed) values for the point. This plot can show the trend of the solution values with regards to matching the weighted observed data. Only those points whose value is specified as observed for the selected data type will be shown in the plot. This plot is not available with transient data. These plots are created in the Plot Wizard by setting the Plot Type to Residual vs. Observed (Weighted). A sample plot is shown in the figure.



Residual vs. Observed Plot Options

After the plot type is set in the First Page of the Plot Wizard, the Next button is clicked to open the Residual vs. Observed (Weighted) Plot Options wizard page. This page contains the following:

Coverage and Measurements

The observation coverage and measurements can be selected for each plot. If only one observation coverage and measurement exist these are used by default.

Use current solution

This option causes the plot to compare the weighted observed values with the residual values of the current solution and time step for each observation point. When the active solution changes, the plot is recomputed and updated. If only one solution is in memory then this option is defaulted.

Use selected solutions

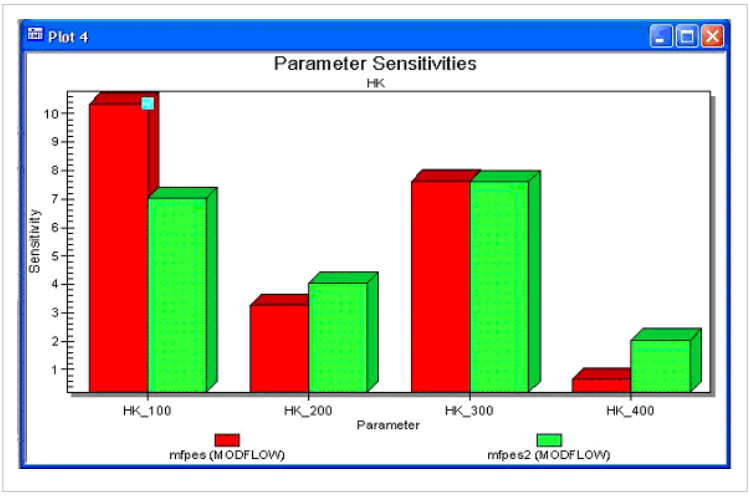
This option causes the plot to compare the weighted observed values with the residual values of the specified solution for each observation point. Changing the active solution does not affect the plot.

Use time step

Because the plot shows only values from a specific time step, The Active Times Step is used by default.

Parameter Sensitivity

A Parameter Sensitivity plot is used to display the sensitivity of the MODFLOW parameters. These plots are created in the Plot Wizard by setting the Plot Type to Paramater Sensitivity. A sample plot is shown in the figure.



Parameter Sensitivity Plot Options

After the plot type is set in the First Page of the Plot Wizard, the **Next** button is clicked to open the Parameter Sensitivity Plot Options wizard page. This page contains the following:

Parameter Type

This option changes the parameter type displayed.

Use current solution

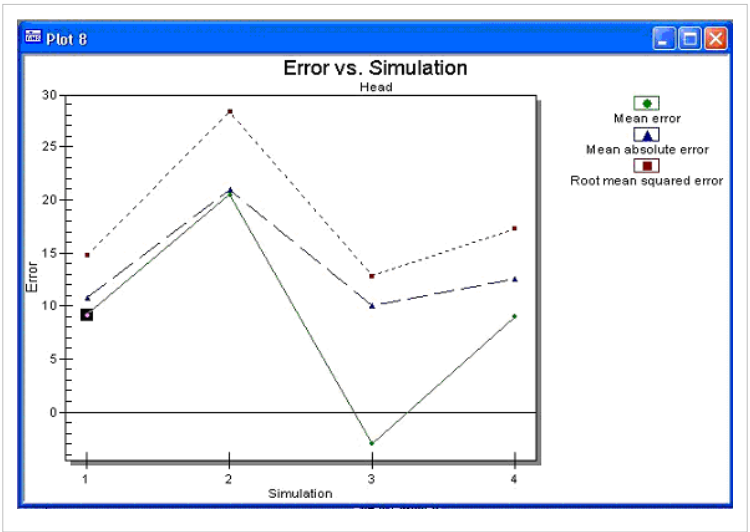
This option causes the plot to compare Parameter Sensitivities of the current solution. When the active solution changes, the plot is recomputed and updated. If only one solution is in memory then this option is defaulted.

Use selected solutions

This option causes the plot to compare Parameter Sensitivities of the specified solution. Changing the active solution does not affect the plot.

Error vs. Simulation

An Error vs. Simulation plot is generally used with steady-state simulations and measurement types. It may be used in transient simulations. This plot can display the mean error, mean absolute error, and root mean squared error between successive solutions and observed data. Various simulations would be run after changing model parameters, such as hydraulic conductivity or recharge. The plot will show trends in the solution to see if model parameter changes are causing better calibration with measured field data. Error vs. Simulation plots are created in the Plot Wizard by setting the Plot Type to Error vs. Simulation. A sample plot is shown in the figure.



Error vs. Simulation Plot Options

After the plot type is set in the First Page of the Plot Wizard, the **Next** button is clicked to open the Error vs. Simulation Plot Options wizard page. This page contains the following:

Solutions

This lists all available solutions.

Move Up/Move Down

GMS initially shows the solutions in the order they were opened. However, this is not necessarily the order in which they were run. To change the order, highlight a solution and move it up or down to rearrange their order.

Observed

This lists all available measurement types that were set up in the Observation Coverage Options dialog, both constant and transient. This plot is generally performed using constant solutions and measurement types, although transient data is allowed. You should select in the combo box the measurement type that you are comparing.

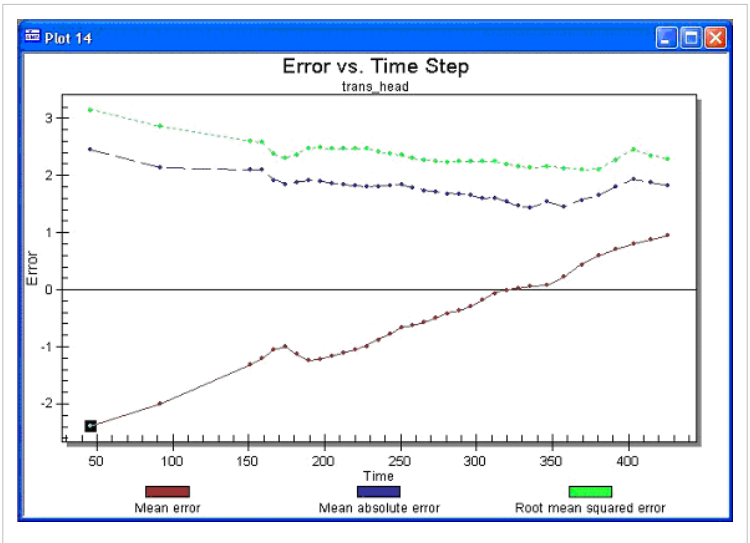
Check Box Options

There are three options that can be turned on or off. They determine whether the mean error, mean absolute error, and root mean squared error plots should be shown. Because these values are an average of all observation points, their line and symbol styles are not linked to any one observation point, but can be defined by clicking on the appropriate canvas window in the dialog.

Error vs. Time Step

An Error vs. Time Step plot is used with transient simulations to display the mean error, mean absolute error, and root mean squared error between a solution and observed data as a function of time. This plot applies to a single Data Set in a model solution. Transient measurement types will show the average errors at each time step of the data set. Error vs. Time Step plots are created in the Plot Wizard by setting the Plot Type to Error vs. Time Step. A sample plot is shown in the figure.

Beginning with version 8.0, this plot can no longer be used with MODFLOW.



Error vs. Time Step Plot Options

After the plot type is set in the First Page of the Plot Wizard, the **Next** button is clicked to open the Error vs. Time Step Plot Options wizard page. This page contains the following:

Use current solution

This option causes the plot to compare Parameter Sensitivities of the current solution. When the active solution changes, the plot is recomputed and updated. If only one solution is in memory then this option is defaulted.

Use selected solutions

This option causes the plot to compare Parameter Sensitivities of the specified solution. Changing the active solution does not affect the plot.

Observed

This lists all available measurement types that were set up in the *Observation Coverage Options* dialog, both constant and transient. A constant measurement should be used for solutions with only one time step, while a transient measurement should be used for transient solutions. You should select the measurement type in the combo box that you are comparing. If only one exists then it is used by default.

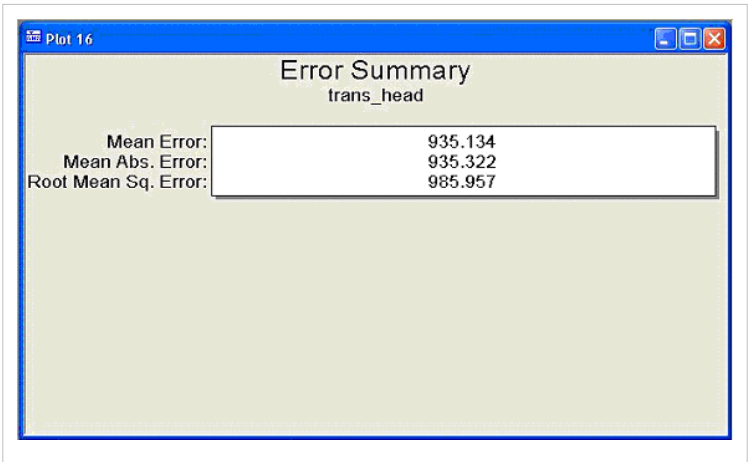
Check Box Options

There are three options that can be turned on or off. They determine whether the mean error, mean absolute error, and root mean squared error plots should be shown. Because these values are an average of all observation points, their line and symbol styles are not linked to any one observation point, but can be defined by clicking on the appropriate canvas window in the dialog.

Error Summary

See the Error Summary Plot page for more details. An Error Summary plot is used to display the mean error, mean absolute error, and root mean squared error for a Solution. Error Summary plots are created in the Plot Wizard by setting the Plot Type to Error Summary. A sample plot is shown in the figure.

Beginning with version 8.0, this plot can no longer be used with MODFLOW. This information can be found by right-clicking on the MODFLOW solution in the Project Explorer.



Error Summary Plot Options

After the plot type is set in the First Page of the Plot Wizard, the **Next** button is clicked to open the Error Summary Plot Options wizard page. This page contains the following:

Use active solution

This option causes the plot to show a summary of mean error between the set of observed values with the values of the active solution for each observation point. When the active solution changes, the plot is recomputed and updated. This option is always on by default at this time

All time steps

This option shows the mean error for all time steps instead of only at the current or specified time step value.

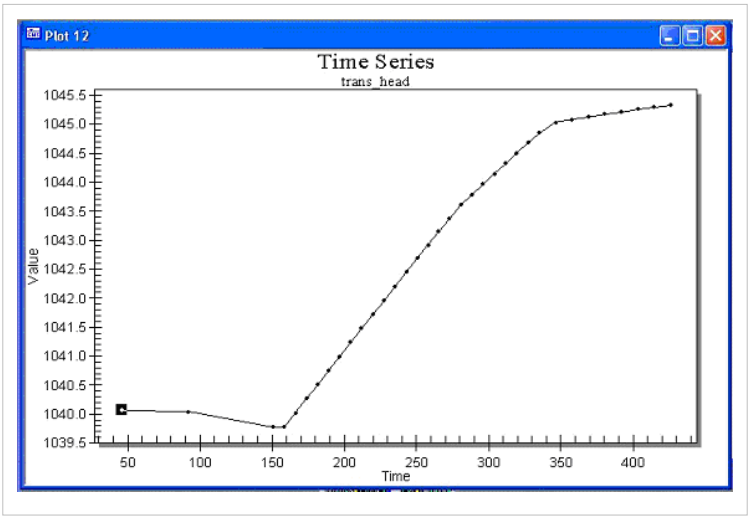
Observed

This section shows the available list of observed values that were set up in the *Observation Coverage Options* dialog. Both constant and transient observed values should be available in this dialog.

Time Series

A Time Series plot is used to display the time variation of one or more scalar Data Sets associated to a given point inside a model solution. In addition, if transient calibration data has been defined, a band can be shown which represents a time variant Calibration Target. Only transient data sets may be used in these plots. Time Series plots are created in the Plot Wizard by setting the Plot Type to Time Series. A sample plot is shown in the figure.

Beginning with version 8.0, these plots have been changed to show observation targets instead of a "band" around the observed data.



Time Series Plot Options

After the plot type is set in the First Page of the Plot Wizard, the Next button is clicked to open the Time Series Plot Options wizard page. This page contains the following:

Coverage and Measurements

The observation coverage and measurements can be selected for each plot. If only one observation coverage and measurement exist these are used by default. All Measurements can also be selected to plot all of the different measurements on one plot.

Use current solution

This option causes the plot to display the values of the active Solution for each observation point being plotted. When the active solution changes, the plot is recomputed and updated. If only one solution is in memory then this option is defaulted.

Use selected solutions

This option causes the plot to display the values of one or more specified Solutions for each point being plotted. Changing the active solution does not affect the plot.

Selected Points

Each of the observation points are shown in a spreadsheet. The show toggle determines which Observation Points will be displayed in a Time Series Plot in the Plot Window. This way, only certain points are plotted in each individual time series plot. All the points can either be turned on or off by selecting the corresponding buttons below the spreadsheet.

Calibration Target

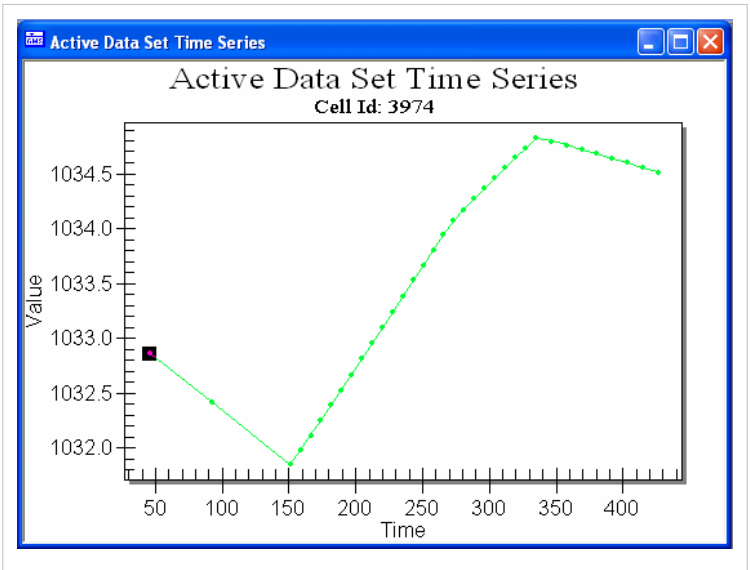
Turn this on to display a band in the plot to define the valid calibration range. If this is turned off, only the calibration curve will be drawn.

Time interval

A starting time and an ending time of observations can be specified by two combo boxes. Only the interval chosen will be shown on the time series plot.

Active Dataset Time Series

A Time Series plot is used to display the time variation of one or more scalar Datasets associated to a given point selected in a model solution. Time Series plots are created in the Plot Wizard by setting the Plot Type to Active Dataset Time Series. A sample plot is shown in the figure.



Active Dataset Time Series Plot Options

After the plot type is set in the First Page of the Plot Wizard, the **Finish** button is clicked to create the active time series plot. For 2D and 3D grids select a grid cell and for 2D and 3D meshes select a node to display the scalar values of the dataset at that location over time. You can select up to five locations to be plotted on one plot.

S/S Flow vs. Time

A Flow vs. Time plot is used to display the flow or water over time for a selected feature object or grid cell. Flow vs. Time plots are created in the Plot Wizard by setting the Plot Type to Flow vs. Time. A sample plot is shown in the figure.

S/S Flow vs. Time Plot Options

After the plot type is set in the First Page of the Plot Wizard, the **Finish** button is clicked to create the flow vs time plot. This plot will report the flow either by selecting a feature object defined as a MODFLOW source/sink in the map module or by selecting a group of cells in the 3D Grid. To change the plot options for the Flow vs Time Plot right-click on the plot and select the ***Plot Data*** command. The *Plot Data* dialog contains the following:

Feature Objects flow

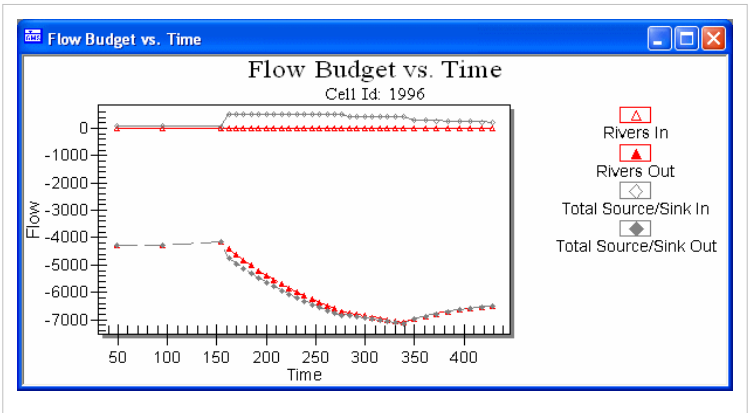
This option allows you to select what data to plot when a Source/Sink feature object is selected in the Map module. By default the computed flow is plotted. If observed values exist for the feature object than those values can also be plotted along with calibration target ranges.

Grid Cell Flow

This option allows you to select what Source/Sink flows to be plotted when Grid Cells are selected in the 3D grid module. The options are: Storage, Constant Head, Drains, General Heads, Rivers, Streams, Recharge, Evapotranspiration, and Total Source/Sink flow in and out of the cells.

Flow Budget vs. Time

A Flow Budget vs. Time plot is used to display the flow or water over time for selected grid cell or for zone budget ids. Flow Budget vs. Time plots are created in the Plot Wizard by setting the Plot Type to Flow Budget vs. Time. A sample plot is shown in the figure.



Flow Budget vs. Time Plot Options

After the plot type is set in the First Page of the Plot Wizard, the **Next** button is clicked to open the Flow Budget Plot Options wizard page. The options on this page are discussed below. The **Finish** button is clicked to create the flow budget vs time plot. This plot will report the flow either by selecting a group of cells in the 3D Grid or by using the zone budget ids.

Display using

This option allows you to determined the data to plot. The Flow budget will be computed either from the selected 3D grid cells or from the selected zone budget ids in the spreadsheet.

Grid Cell Flow

This option allows you to select what Source/Sink flows to be plotted. The options are: Storage, Constant Head, Drains, General Heads, Rivers, Streams, Recharge, Evapotranspiration, and Total Source/Sink flow in and out of the cells.

Gage Package Value vs. Time

This plot shows a time series for a single gage package column. After the plot type is set in the First Page of the Plot Wizard, the Next button is clicked to open the Gage Package Time Series wizard page. To generate a gage plot the gage file needs to be selected from the list on the left, and the data column from the list on the right. If GMS is unable to properly read the data from the gage file, an error is shown in the wizard page to the right of the data column list.

Finish

When the Finish button is selected, a window is opened with the plot. Plot windows are created each time the Plot Wizard is run. See the 2D Plots discussion for information on editing plots that have been created.

Right-Click Menu Commands

Once the plot has been created, the appearance and data of the plot can be altered with commands accessed by right-clicking on the plot window. The commands available through the right-click menu are described below.

Plot Data – The plot data command brings up the second step of the plot wizard where the attributes of each plot are set. The plot data can be updated based upon the type of plot. For Histogram plots it brings up a dialog used to edit the precision displayed on the plot.

Display Options – The Display Options command allows you to change general display attributes of the plot (Border Style, Precision, Axis type, Fonts, Colors, etc.).

Axis Titles – The axis titles menu is used to change the x and y axis titles.

Set As Display Defaults – To save the plots current settings as the default settings, select the Save Settings menu item.

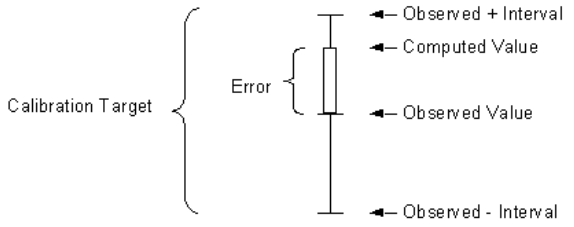
Legends – The legend can be turned on by right clicking on the plot and selecting a location from the Legend submenu. The maximum number of points included in the legend depends upon the size of the plot window.

Export/Print – By selecting on the Export/Print menu item, a dialog is displayed showing options for printing or exporting the plots values.

Default Display – To save the plots current settings as the default settings, select the Save Settings menu item.

View Values – To view the values of the plot in a spreadsheet format, select the View Values menu. A spreadsheet containing the data points associated with the current plot appear.

Calibration Targets



Example of a calibration target

If an observed value has been assigned to an observation point or if an observed flow has been assigned to an arc or polygon, the calibration error at each object can be plotted using a "calibration target". A set of calibration targets provides useful feedback on the magnitude, direction (high, low), and spatial distribution of the calibration error.

The components of a calibration target are illustrated in the following figure. The center of the target corresponds to the observed value. The top of the target corresponds to the observed value plus the interval and the bottom corresponds to the observed value minus the interval. The colored bar represents the error. If the bar lies entirely within the target, the color bar is drawn in green. If the bar is outside the target, but the error is less than 200%, the bar is drawn in yellow. If the error is greater than 200%, the bar is drawn in red. The display options related to calibration targets are specified in the *Feature Object Display Options* dialog.

If the active time step is before the first observed time, or after the last observed time, the targets are drawn lighter.

Model Checker

Once a mesh or grid is generated and all of the analysis options and boundary conditions have been specified, the next step is to save the simulation to disk and run the model. However, before saving the simulation and running the model, the model should be checked with the Model Checker. Because of the significant amount of data required for a simulation for all the different models, it is often easy to neglect important data or to define inconsistent or incompatible options and parameters. Such errors will either cause the model to crash or to generate an erroneous solution. The purpose of the Model Checker is to analyze the input data currently defined for a model simulation and report any obvious errors or potential problems. Running the Model Checker successfully does not guarantee that a solution will be correct. It simply serves as an initial check on the input data and can save a considerable amount of time that would otherwise be lost tracking down input errors.

Running the Model Checker

To check the current data, select the ***Check Simulation*** command from the "current model" menu. The *Model Checker* dialog will appear. To run the Model Checker, select the button labeled **Run Check** at the top of the dialog. This generates a list of possible errors and warning messages in the top scrolling window.

If the model checker finds any potential errors with your input, then fix the errors and rerun the model checker.

Options

The Checker Options button in the Model Checker allows you to customize the checks that will be performed. A check box is provided for each category of the model input data. Turning off any of the options will suppress the warnings and errors associated with these categories. Also provided is the option to define the maximum number of errors and warnings to be reported of the same type. Messages classified as warnings can also be suppressed.

Save Messages

The Save Messages button provides the option to save the current listing of warnings and error messages to a text file.

One unique feature of the MODFLOW Model Checker is the Fix Layer Errors option.

7.2. Parameters

Parameters

A parameter is a variable that is used to control one or more other values. GMS uses parameters with MODFLOW to define inputs for forward runs or for model calibration or for stochastic modeling.

Key value and standard MODFLOW parameters

There are two ways to do MODFLOW parameterization in GMS:

- The key value method (recommended)
- The standard MODFLOW method

Key values

Key values are used to parameterize the MODFLOW input. Key values can be used for both the zonation and pilot points methods of defining parameters. A key value is a number that is assigned as input that marks the input values as belonging to a parameter. When selecting a key value, a number should be chosen that is not likely to occur in typical input for that parameter. We recommend using negative numbers in most cases.

For example, a model may have four K zones and three recharge zones. The four K zones would be marked by assigning -100, -200, -300, and -400 to the cells in the K array for each of the four zones. Likewise, the recharge zones would be marked by assigning -500, -600, and -700 to the appropriate cells in the recharge array.

Key values can be assigned either by editing the cell array values directly in the 3D grid module or by assigning the values to a set of polygons or arcs in the conceptual model and selecting the ***Map → MODFLOW*** command.

When MODFLOW is running and data is read from the HDF5 file, if one of the parameter key values is found in the data then the parameter value is substituted into the array or list.

The key value approach makes it much easier to support transient parameters and very large sets of pilot points. Also, this approach allows GMS users to use parameters with the BCF package. This feature is not available with the MODFLOW PES process.

Standard MODFLOW parameters

The "key value" approach is the preferred approach to defining parameters in GMS. Using key values is the only option for WEL, RIV, DRT, DRN, GHB, CHD, STR, and HFB parameters. In GMS, using the key value approach with these parameters provides the same functionality of parameter instances available in MODFLOW.

Key values can also be used with array based parameters. However, GMS does support defining array based parameters with clusters and instances (for ETS, EVT, RCH parameters).

When reading in a MODFLOW simulation that was created outside of GMS all parameters will be converted to key values so long as the parameter can be represented by key values.

Key values can not be used to represent an array based parameter if the parameter is defined using more than one cluster or more than one instance. Also, if more than one parameter uses the same zone array with a matching IZ value then the parameter can not be represented using key values. Further, if the multiplier array associated with the parameter has values other than 1.0 in the zones where the parameter is used then the parameter can not be represented with key values.

The standard MODFLOW method is considered an "advanced" feature in GMS. **Only users that understand how MODFLOW uses parameters should attempt to use this feature.**

For more information, refer to the Standard MODFLOW Parameters page.

Using parameters

To use parameters, you must:

1. Parameterize your model and
2. Create a parameter list

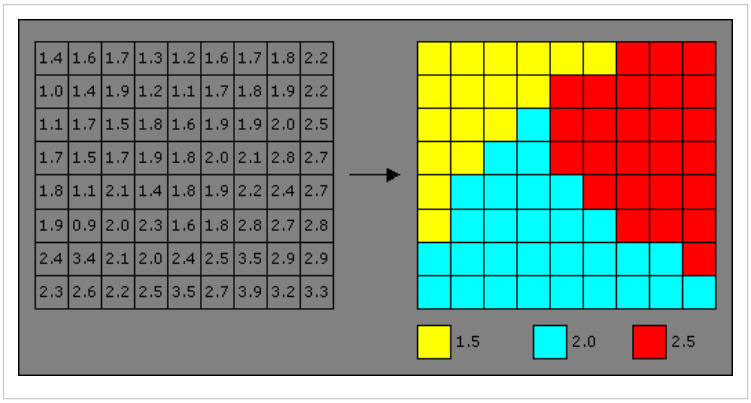
Parameterizing the model

There are two methods used to parameterize a model:

- Zonation
- Pilot Points

Zonation

The most common form of parameterization is zonation. With this approach, an array of input values is divided into zones where all of the cells in each zone share a single parameter value. This concept is illustrated in the figure below. The entire array of values is represented by three parameters.



Zonation is most easily accomplished in GMS by assigning key values to polygons in the map module. It can also be accomplished by assigning key values to a selected set of cells in the 3D grid module using the ***Cell Attributes*** command.

Pilot points

Another way to parameterize a model is to use pilot points. For more information on pilot points, refer to the Pilot Points page.

Creating a parameter list

The list of parameters is defined using the *Parameter* Dialog. In general, the number of parameters should be less than the number of observations. However, if the user chooses to use pilot points with PEST in regularization mode, then the number of parameters does not have to be less than the number of observations.

Legal MODFLOW Parameters

The following MODFLOW input values can be defined as parameters in GMS:

Package	Option
LPF/HUF	• HK – Horiz. hydraulic conductivity • HANI – Horiz. anisotropy • VK – Vert. hydraulic conductivity • VKCB – Vert. hydraulic conductivity of confining beds • VANI – Vert. anisotropy • SS – Specific storage • SY – Specific yield
Recharge	RCH – Recharge value
Evapotranspiration	EVT – Max ET flux
Evapotranspiration Segments	ETS – Max ET flux
Well	WELL – Pumping rate
River	RIV – River conductance
General Head	GHB – Conductance
Drain	DRN – Conductance
Time-Variant Specified-Head	CHD – Head
Stream	STR – Conductance
Stream-flow Routing	SFR – Conductance
Horizontal Flow Barrier	HFB – Hydraulic characteristic

Parameter Dialog

When building a MODFLOW inverse model, the input data must be parameterized. This is accomplished by assigning a set of key values to selected input fields. Once the key values are assigned, the next step is to create a parameter list.

Parameters can also be used to perform forward runs.

See also Standard MODFLOW Parameters.

Creating/Deleting Parameters

The *Parameters* dialog contains the list of parameters. A new parameter can be created by selecting the **New Parameter** button. Each parameter that is defined should correspond to a key value that has been defined in the MODFLOW input. A parameter can be removed from the list by selecting the parameter and selecting the **Delete Parameter** button. The entire list of parameters can be deleted by selecting the **Delete All** button.

Initialize from Model

In most cases, the fastest and simplest way to create the parameter list is to use the **Initialize from Model** button. When this button is selected, GMS traverses the MODFLOW input data corresponding to legal parameter values and searches for key values. It is assumed that the key values are entered as negative numbers. When a unique negative number is found, a new parameter is added to the list, and a default name is given to the parameter based on the parameter type.

NOTE: The ***Initialize from Model*** command will not search for key values in the Well package. This is because negative pumping rates are perfectly common and do not necessarily correspond to key values. If you wish to define a well Q as a parameter, you should use the **New Parameter** button and manually create the parameter.

Import Optimal Values

After performing an inverse model run, the inverse code writes out a text file containing the set of optimal parameter values corresponding to the minimum calibration error. The next step is to read these values into GMS. This is accomplished by selecting the **Import Optimal Values** button. Once you open the file, the optimal parameter values will be loaded into the starting value field and displayed in the parameter list.

If any of your parameters use pilot points, importing the optimal values will also import and create a new dataset for the associated 2D scatter point set.

Spreadsheet

The spreadsheet holds parameters, their types, starting and bounding values and other options that depend on the packages and run options defined for the current MODFLOW simulation in the Global Options\Basic Package.

Parameter Estimation Solve

Toggle on this option to solve for the optimal parameter value using a parameter estimation program like PEST. (See Automated Parameter Estimation)

Name

The name must be unique and limited to 8 characters. The default name should be sufficient. This name will be used to reference the parameter in the MODFLOW solution and output files.

Key

The key value, usually a negative value, must be unique and is used to link the parameter with the data in the MODFLOW input files. The key value should also be entered into the MODFLOW data by directly entering the values using the grid based approach or by using the map module.

Type

GMS supports most of the parameter types that are also supported by the MODFLOW PES process.

Start Value/Pilot Points

This value will be the starting value for inverse modeling, the mean value for stochastic modeling, or the substitute value for forward runs.

For inverse modeling, the closer the starting value is to the "optimal" value, the better the odds that the inverse model will converge and the less time it will take to converge. It is generally not a good idea to give all parameters of a given type (e.g., recharge) a constant value and let the inverse model start from that point. Ideally, field tests, soil types, ground cover, and sound modeling judgement can provide a good set of starting values. It is also a good idea to undergo some manual trial-and-error calibration prior to setting up the inverse code.

Pilot points can be used to define a parameter by selecting the drop-down arrow in this column and selecting the **Pilot points** option. Pilot points are an alternative to using zonation to define parameter locations. When you use pilot points, you use the **Pilot Point Options** button to choose a 2D point scatter point set and choose the appropriate interpolation options.

Min Value Max Value

The min and max values will provide the bounds for the parameter, and they must encompass the starting value. The parameter values will be forced between these values during inverse and stochastic modeling. In these cases, the min and max values are just "suggestions" and are used to predict parameter values.

When selecting the min and max values for the parameters, care should be taken not to make the range in values too large. Inverse models are highly senstive to the stability of the underlying model. If MODFLOW does not converge, the invese model will not be able to find a solution. Furthermore, excessive cell drying can cause the inverse model to fail to converge. If the min and/or max values are too extreme, the odds of the MODFLOW model not converging or excessive numbers of cells going dry increases. It is best to select a limited range for each parameter and then to compare the final optimal parameter value to this range. If the optimal value is at either the min or max of the range, the range can be adjusted and the inverse model can be re-launched.

Log xform

This option log transforms the value during prediction process of inverse modeling and the random number generation process of stochastic modeling. The best parameters to log transform are those that can vary by orders of magnitude like hydraulic conductivity.

It is also recommended that you log transform recharge parameters if you are using pilot points for hydraulic conductivity and the hydraulic conductivity parameter is log transformed.

BSCAL

MODFLOW documentation includes:

This value is an alternate scaling factor for the parameter, and always needs to be a positive number. If the parameter value becomes 0.0, which can occur for parameters that are not log transformed, BSCAL is used in the scaling. If the absolute value of the parameter is less than BSCAL, BSCAL is used in the scaling. The best value to use is problem dependant. Good choices are the smallest reasonable value of the parameter or a value two to three orders of magnitude smaller than the value specified by the starting value. If the smallest reasonable value is 0.0, a reasomable non-zero value needs to be used. BSCAL has no effect on the scaled sensitivities for log-transformed parameters.

Multiplier

Select this option to include a multiplier array for RCH and HK parameters.

Dataset / Folder

Use this button to select a multiplier array of a set of multiplier arrays (stochastic only) by selecting a folder of datasets.

Stochastic Options

Standard Deviation

Use this field to specify the standard deviation of a parameter for a stochastic simulation.

Mean value

Use this field to specify the mean of a parameter for a stochastic simulation.

Distribution

When the parameter is stochastic, use this option to choose between a normal or linear distribution. A random number for the parameter is generated using the distribution, the mean value (starting value) and the standard devation.

Std Deviation

The standard deviation is used for a stochastic parameter to generate a random number using the chosen distribution.

Num Segments

When the parameter is stochastic and the stochastic method is Latin Hypercube, the number of segments helps determine how man total MODFLOW runs will be used.

Pilot Points

Pilot points can be thought of as a 2D scatter point set. Instead of creating a zone and having the inverse model estimate one value for the entire zone, the value of the parameter within the zone is interpolated from the pilot points. Then the inverse model estimates the values at the pilot points. The figure below shows a set of pilot points used to estimate horizontal hydraulic conductivity. Notice how the hydraulic conductivity now varies from cell to cell. When the inverse model runs, the values at the pilot points are adjusted and the "surface" defining the variation of K values is warped until the objective function is minimized.

PEST provides an additional option for the pilot point method called "regularization". Regularization imposes an additional measure of "stiffness" to the parameter being interpolated via a "homogeneity" constraint. In the absence of any strong influence from the PEST objective function, this constraint causes values at pilot points to approximate the mean value of adjacent pilot points. This constraint makes the inversion process much more stable and makes it possible to violate one of the typical constraints associated with parameter estimation: namely, the requirement that the number of parameters must be less than the number of observations. With regularization, the number of parameters can greatly exceed the number of observations. As a result, complex hydraulic conductivity distributions can be defined, resulting in extremely low residual error. The pilot point method with regularization is an incredibly powerful feature of PEST. (For more on PEST see Automated Parameter Estimation)

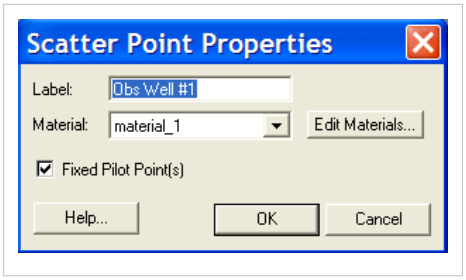
Pilot Points and Resulting Conductivity Field

Interpolation Options

Kriging and IDW are the only interpolation options supported with pilot points. The kriging option requires the establishment of a model variogram (by creating a nested structure). The nodal function options in the IDW method are not supported because those schemes compute gradients based on the data set values at the surrounding points. With the pilot point method, the values at the points will change during the inversion process, thereby rendering the previously computed gradients inaccurate.

Pilot Point Conditioning

For pilot point interpolation of hydraulic conductivity, it is sometimes useful to include one or more measured K values with the pilot point set. These measured values could represent K values extracted from a field pump test. The *Pilot Point Conditioning* option is available to represent this scenario. One of the properties associated with scatter points is a *Fixed pilot point* toggle. If this toggle is on and the corresponding scatter point set is used for pilot point interpolation, the K value assigned to the point is not allowed to vary during the parameter estimation process.



Guidelines for Placement of Pilot Points

Note: The recommended maximum number of pilot points is about 200.

1. Place points between observations rather than on top of observations
2. Add greater density where there are more observations
3. Add points where head gradient is steep
4. Place a row of points between observation wells and head-dependent boundaries
5. Fill in the gaps

Multiplier Arrays for Parameters

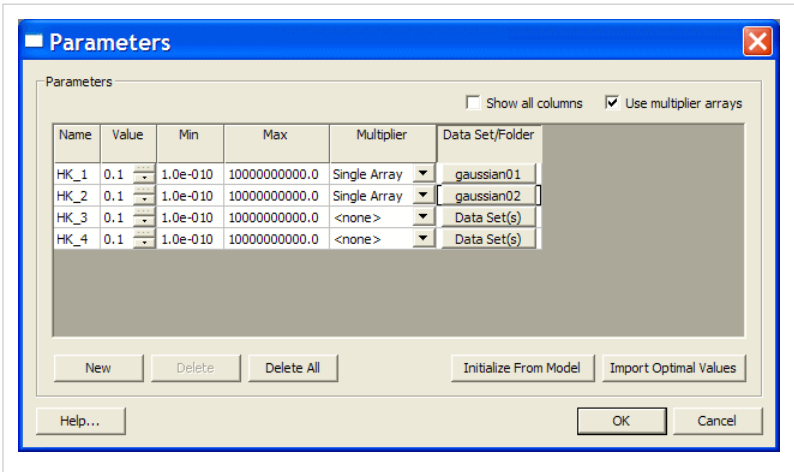
HK and RCH parameters may be associated with a multiplier array. A dataset is associated with a parameter zone and the starting parameter value is multiplied by the data set to define the spatial variation of the parameter throughout the zone.

Setting up Multiplier Arrays

The multiplier dataset is associated with the parameter zone in the Parameters dialog by first turning on the **Use multiplier arrays** toggle, selecting either **Single Array** or **Multiple Array** from the pull-down list in the **Multiplier** column, and then selecting the data set using the button in the **Dataset/Folder** column. If the **Single Array** option is selected, a single dataset should be selected in the Dataset/Folder column. If the **Multiple Array** option is selected, an entire folder of datasets should be selected. The **Multiple Array** option is only available for stochastic modeling.

If the **Single Array** option is selected the array for the parameter will be defined as the starting/mean value multiplied by the multiplication array for all cells associated with the parameter. Multiplier arrays are not available for parameters that use pilot points.

When the **Multiple Arrays** Option is selected, the number of stochastic model runs will be a function of how many datasets are in the folder selected by the user for the multipliers.



Guassian Field Based Monte Carlo Simulations

The **Multiple Array** option for user-defined multiplier arrays can be used in combination with the new Gaussian Field Generator to perform a Monte Carlo simulation. This is accomplished by first generating a set of Gaussian fields using the FIELDGEN code and then associating the resulting folder of datasets with a parameter as described above. A stochastic simulation can then be performed using the Parameter Randomization method. For each model instance, GMS loads a new instance of the multiplier array into the model input. A default parameter value of 1.0 is

generally recommended in such instances.

Standard MODFLOW Parameters

Caution

There are two ways to do MODFLOW parameterization in GMS:

1. The key value method **(recommended)**
2. The standard MODFLOW method

The "key value" approach is the preferred approach to defining parameters in GMS. Using key values is the only option for WEL, RIV, DRT, DRN, GHB, CHD, STR, and HFB parameters. In GMS, using the key value approach with these parameters provides the same functionality of parameter instances available in MODFLOW.

Key values can also be used with array based parameters. However, GMS does support defining array based parameters with clusters and instances (for ETS, EVT, RCH parameters).

When reading in a MODFLOW simulation that was created outside of GMS all parameters will be converted to key values so long as the parameter can be represented by key values.

Key values can not be used to represent an array based parameter if the parameter is defined using more than one cluster or more than one instance. Also, if more than one parameter uses the same zone array with a matching IZ value then the parameter can not be represented using key values. Further, if the multiplier array associated with the parameter has values other than 1.0 in the zones where the parameter is used then the parameter can not be represented with key values.

The standard MODFLOW method is considered an "advanced" feature in GMS. **Only users that understand how MODFLOW uses parameters should attempt to use this feature.**

This article describes how to use the standard MODFLOW parameterization method in GMS.

Support in GMS

Reading

GMS can read MODFLOW models that use standard MODFLOW parameters.

Writing

GMS writes MODFLOW models using the key value approach. So, although GMS can read models that use standard MODFLOW parameters, it cannot write them using the standard MODFLOW parameter method. Writing is usually done using the key value method. There are a few exceptions which include recharge and evapotranspiration parameter instances, and LPF and HUF parameter clusters. GMS will write these parameters using the standard MODFLOW parameter method because these cannot always be represented using the key value method.

Editing

When GMS reads a model that uses standard MODFLOW parameters it converts them to regular GMS key value approach parameters. The parameters can then be edited using the *Parameters* Dialog. Recharge, evapotranspiration, LPF, and HUF parameters are special in that you can edit the instance and cluster information associated with these types of parameters.

MODFLOW Parameter Clusters Dialog

The *MODFLOW Parameter Clusters* Dialog allows users to define instances for RCH, EVT, LPF, and HUF parameters that use clusters. The inputs in this dialog basically follow the necessary inputs for defining a parameter instance in a package file. You may wish to review the MODFLOW Parameter Clusters and Instances section below.

Array based parameters are defined using clusters. A cluster is a multiplier array, a zone array, and specified zone values where the parameter is applied. Multiplier arrays and zone arrays have associated datasets underneath the three dimensional grid in the Project Explorer.

Instances are enabled for RCH and EVT parameters. Instances allow the user to define multiple sets of clusters that are all tied to one parameter. Then the user may use different instances in different stress periods in their MODFLOW model. For more information on parameter instances consult the MODFLOW documentation.

In the MODFLOW Parameters dialog the user selects the **Define clusters** option for a parameter. This will allow the user to specify the number of instances and clusters that are used to define the parameter.

In the *Parameter Instances* dialog the user defines a name for each parameter instance for RCH and EVT parameters. For LPF parameters a level is defined and for HUF parameters a hyrdogeologic unit is defined. Then for each cluster the user selects a multiplier array and a zone array. These are datasets on the 3D Grid. The user must also specify the zone values (IZ) where the parameter is to be applied in the model. If there is more than one IZ value for the cluster then the user enters the numbers with spaces between the entries. So if the parameter is to be applied where the zone array values are 1 and 3 then the user would enter "1 3". The user must also specify the stress periods where an instance is to be used. The numbers entered in the Stress Periods field should also be space delimited. This means if you want an instance to be used in stress periods 1, 2, and 5 then your entry in the Stress Periods field should be "1 2 5".

When the package is written out for MODFLOW the instances will be included in the parameter definition and used for forward runs or for parameter estimation runs.

MODFLOW Parameter Clusters and Instances

For those wanting to follow the standard MODFLOW approach to parameterization, the following explanation may be helpful. You should refer to the MODFLOW documentation for more information.

Definitions

Here is a brief review of the most important terms used when dealing with parameters.

- *Parameter* – Has a name, type, one or more clusters, and zero or more instances.
- *Parval* – The value of the parameter.
- *Cluster* – Has a multiplier array (*Mltarr*), a zone array (*Zonarr*), and zone numbers (*IZ*).
- *Mltarr* – Name of the multiplier array. Parval is multiplied by this to define the value.
- *Zonarr* – Name of the zone array used to define the cells that are associated with a parameter.
- *IZ* – Up to 10 zone numbers (separated by spaces) that define the cells that are associated with a parameter.
- *Instance* – Parameter cluster that could be used for different stress periods in a MODFLOW simulation.

Examples

Below are some examples showing different ways parameters can be used. The examples use parameters to define recharge for a forward run (not doing inverse modeling). The grid in the examples is 5 rows, 5 columns, 1 layer. The examples use the following multiplier and zone arrays.

Multiplier arrays

MULT0001

1.0	1.0	1.0	1.0	1.0
1.0	1.0	1.0	1.0	1.0
1.0	1.0	1.0	1.0	1.0
1.0	1.0	1.0	1.0	1.0
1.0	1.0	1.0	1.0	1.0

MULT0002

0.5	0.5	0.5	0.5	0.5
0.5	0.5	0.5	0.5	0.5
0.5	0.5	0.5	0.5	0.5
0.5	0.5	0.5	0.5	0.5
0.5	0.5	0.5	0.5	0.5

Zone Arrays

ZONE0001

2	2	2	0	0
2	2	2	0	0
2	2	2	0	0
0	0	0	0	0
0	0	0	0	0

ZONE0002

3	3	3	3	3
3	3	3	3	3
4	4	4	4	4
4	4	4	4	4
5	5	5	5	5

ZONE0003

0	0	0	0	0
0	0	6	7	0
0	0	6	7	0
0	0	0	0	0
0	0	0	0	0

Example 1

Steady state. 1 recharge parameter with 1 cluster, 1 instance.

Recharge file	Variables	Explanations
`PARAMETER 1`	`PARAMETER NPRCH`	`One recharge parameter will be used`
`3 40`	`NRCHOP IRCHCB`	`Apply to highest active cell, save CCF to unit 40`
`Param1 RCH 0.00005 1`	`PARNAM PARTYP Parval NCLU`	`Parameter name, type, value and number of clusters`
`MULT0001 ZONE0001 2`	`Mltarr Zonarr IZ`	`Multiplier array, zone array, and zone number`
`1 1`	`INRECH INIRCH`	`One parameter used in current stress period, INIRCH (ignored)`
`Param1`	`Pname`	`Name of parameter used to define RECH in this stress period`

Results

The resulting recharge applied to the top-most active layer would be:

0.00005	0.00005	0.00005	0	0
0.00005	0.00005	0.00005	0	0
0.00005	0.00005	0.00005	0	0
0	0	0	0	0
0	0	0	0	0

Example 2

Steady state. 2 recharge parameters:

- the first with 1 cluster, 1 instance
- the second with 2 clusters, 1 instance.

Recharge file	Variables	Explanations
PARAMETER 2	PARAMETER NPRCH	Two recharge parameters will be used
3 40	NRCHOP IRCHCB	Apply to highest active cell, save CCF to unit 40
Param1 RCH 0.00005 1	PARNAM PARTYP Parval NCLU	Parameter name, type, value and number of clusters
MULT0001 ZONE0001 2	Mltarr Zonarr IZ	Multiplier array, zone array, and zone number
Param2 RCH 0.00004 2	PARNAM PARTYP Parval NCLU	Parameter name, type, value and number of clusters
MULT0002 ZONE0002 4 5	Mltarr Zonarr IZ	Multiplier array, zone array, and zone numbers
MULT0002 ZONE0003 6 7	Mltarr Zonarr IZ	Multiplier array, zone array, and zone numbers
2 1	INRECH INIRCH	Two parameters used in current stress period, INIRCH (ignored)
Param1	Pname	Name of parameter used to define RECH in this stress period
Param2	Pname	Name of parameter used to define RECH in this stress period

Results

The intermediate results for each parameter cluster are listed below:

Param1

0.00005	0.00005	0.00005	0	0
0.00005	0.00005	0.00005	0	0
0.00005	0.00005	0.00005	0	0
0	0	0	0	0
0	0	0	0	0

Param2, cluster 1

0	0	0	0	0
0	0	0	0	0
0.00002	0.00002	0.00002	0.00002	0.00002
0.00002	0.00002	0.00002	0.00002	0.00002
0.00002	0.00002	0.00002	0.00002	0.00002

Param2, cluster 2

0	0	0	0	0
0	0	0.00002	0.00002	0
0	0	0.00002	0.00002	0
0	0	0	0	0
0	0	0	0	0

The final result after accumulating each cluster is:

0.00005	0.00005	0.00005	0	0
0.00005	0.00005	0.00007	0.00002	0
0.00007	0.00007	0.00009	0.00004	0.00002
0.00002	0.00002	0.00002	0.00002	0.00002
0.00002	0.00002	0.00002	0.00002	0.00002

Example 3

Transient. 1 recharge parameter with 1 cluster, 2 instances. One instance is used in the first and third stress periods, and the other is used in the second stress period.

Recharge file	Variables	Explanations
PARAMETER 1	PARAMETER NPRCH	One recharge parameters will be used
3 40	NRCHOP IRCHCB	Apply to highest active cell, save CCF to unit 40
Param1 RCH 0.00005 1 INSTANCES 2	PARNAM PARTYP Parval NCLU INSTANCES NUMINST	Parameter name, type, value number of clusters, number of instances
Instance1	INSTNAM	Instance name
MULT0001 ZONE0001 2	Mltarr Zonarr IZ	Multiplier array, zone array, and zone number
Instance2	INSTNAM	Instance name
MULT0002 ZONE0001 2	Mltarr Zonarr IZ	Multiplier array, zone array, and zone number
1 1	INRECH INIRCH	One parameters used in current stress period, INIRCH (ignored)
Param1 Instance1	Pname Iname	Name of parameter and name of instance used in this stress period
1 1	INRECH INIRCH	One parameters used in current stress period, INIRCH (ignored)
Param1 Instance2	Pname Iname	Name of parameter and name of instance used in this stress period
1 1	INRECH INIRCH	One parameters used in current stress period, INIRCH (ignored)
Param1 Instance1	Pname Iname	Name of parameter and name of instance used in this stress period

Results

The intermediate results for each parameter cluster are listed below:

Stress Period 1, Param1, Instance RCH_1_1

0.00005	0.00005	0.00005	0	0
0.00005	0.00005	0.00005	0	0
0.00005	0.00005	0.00005	0	0
0	0	0	0	0
0	0	0	0	0

Stress Period 2, Param1, Instance RCH_1_2

0.000025	0.000025	0.000025	0	0
0.000025	0.000025	0.000025	0	0
0.000025	0.000025	0.000025	0	0
0	0	0	0	0
0	0	0	0	0

Stress Period 3, Param1, Instance RCH_1_1

0.00005	0.00005	0.00005	0	0
0.00005	0.00005	0.00005	0	0
0.00005	0.00005	0.00005	0	0
0	0	0	0	0
0	0	0	0	0

7.3. Stochastic Modeling

Stochastic Modeling

There are two methods in GMS for stochastic modeling using MODFLOW 2000. The first, parameter zonation, uses either a Random Sampling, Latin Hypercube Sampling, or Gaussian Fields to generate the different realizations. The second approach uses indicator simulations generated by T-PROGS.

After the stochastic simulation results are generated, you can view these results using the Project Explorer. You can also refine the results by using the Risk Analysis Wizard or Statistical Analysis of Stochastic solutions.

Stochastic Applications

One approach for dealing with model heterogeneity is stochastic simulations based on multiple equally plausible candidate realizations of the site heterogeneity. Ideally, such an approach would enable the generation of variability in subsurface soil stratigraphy based on interpretable geologic parameters such as lens width, material proportions, juxta-positioning tendencies and anisotropy. Multiple realizations that are conditioned to borehole data provide modelers with a rational approach for dealing with uncertainty associated with site characterization. Stochastic simulations can be applied to regional representations of the aquifer behavior in addition to local scale simulations. Stochastic simulations are particularly well-suited to local scale models since the resulting complex heterogeneity is more representative of actual stratigraphic deposition. This heterogeneity makes realistic and potentially more accurate contaminant transport simulation possible by simulating the preferential flow channels resulting from thin lenses of clays, sands, or other materials. The ultimate result of a stochastic approach is multiple simulations of hydraulic parameters that create a probabilistic solution. Such a solution has more credence and provides a better understanding of actual site conditions.

The ultimate application of T-PROGS is to generate stochastic simulations of soil heterogeneity. These realizations can then be incorporated into MODFLOW simulations as "material sets" in the LPF package or as "HUF data" in the HUF package. (See T-PROGS)

Stochastic Inverse Modeling

Stochastic inverse modeling is a MODFLOW run option that takes each run in a stochastic simulation and performs parameter estimation on the run to find the optimal values based on observation data. This option is very time consuming compared with a regular stochastic simulation and a parameter estimation run because you are doing parameter estimation for each stochastic run times.

Stochastic inverse modeling can be performed only when using material sets or HUF arrays as chosen in the *Stochastic Options* dialog. PEST is the parameter estimation code supported by GMS.

The following occurs during the stochastic inverse process:

1. Run MODFLOW for the stochastic simulation iteration.
2. Set the starting head equal to the resulting heads from the MODFLOW run.
3. Run parameter estimation.
4. Run final MODFLOW (if needed for PEST).
5. Move to next stochastic simulation iteration.

The starting heads are interpolated to decrease the run times during the inverse portion.

Stochastic Options Dialog

You use the stochastic options dialog to select the type of stochastic simulation its major options.

Parameter Randomization

This option uses parameters defined in *Parameters* Dialog.

Material Sets

This option becomes available when there is at least one material set simulation in memory. One method for creating material sets is to use T-PROGS. When this stochastic option is chosen, MODFLOW will be run once for each material set. This option also requires that the LPF package and the material IDs option be chosen.

HUF Sets

This option becomes available when there is at least one HUF set simulation in memory. One method for creating HUF sets is to use T-PROGS. When this stochastic option is chosen, MODFLOW will be run once for each HUF set. This option also requires that the HUF package be chosen.

Only Save Solutions

With this option selected, during each stochastic iteration, changes are made to MODFLOW simulation and only a few files are saved. If this option is not selected, each stochastic iteration results in a new entire set of MODFLOW files being saved.

Using this option requires less disk space, but doesn't allow you to load and rerun individual stochastic iteration simulations.

Using Parameter Zonation With Stochastic Modeling

To create a stochastic MODFLOW simulation using parameter zonation, you follow these steps:

- First define your zones using key values.
- Define parameters that link with your zones.
- Select the **Stochastic Simulation** option from the *Global Options* dialog.
- Select the Parameter Randomization option from the *Stochastic Options* dialog.
- Choose whether you want to use the Random Sampling or Latin Hypercube randomization approaches in the *Parameters* dialog.
- Save and Run your model.
- View the different model results using the Project Explorer.
- Further analyze the results using the Risk Analysis Wizard.

Random Sampling

Random Sampling is the most widely used approach for generating multiple random model simulations. GMS supports both normal and uniform distributions.

A normal distribution can be defined as:

$$f(x) = \frac{1}{\sqrt{2\pi\sigma}}\exp\left(-\frac{(x-u)^2}{2\sigma^2}\right)$$

where σ is the standard deviation, μ is the mean, and x is the value being sampled. A uniform distribution can be defined as:

$$f(x) = \frac{1}{\beta - \alpha}$$

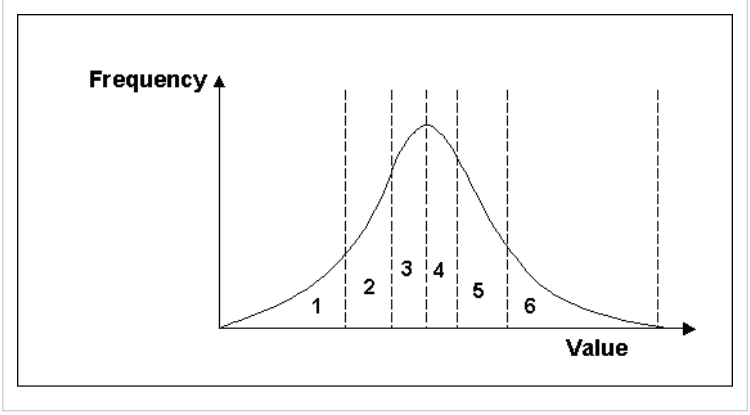
where α and β are the bounds of the parameter value x.

To set up the Random Sampling, you need to specify the mean, standard deviation, and upper and lower bounds for each parameter. Finally, you choose how many realizations you want to generate.

Latin Hypercube

The Latin Hypercube randomization approach is a method that tries to efficiently probe the probability space for each parameter in a simulation in such a way that there is at least one simulation that represents every probability area for each parameter.

First, we specify the number of segments for each parameter. The total probability, defined by a distribution, mean, standard devation, and upper and lower bounds, is divided up into parts with equal probability (area). GMS then generates a random parameter value so that there is one value that lies within each probability segment.



This is repeated in a combinatorial fashion for each parameter so that there are

$$\prod_{i=1}^{n} P_i$$

number of simulations, where n is the number of parameters and P is the number of segments for the ith parameter. For example, if there were three parameters with four, four, and five segments, the number of model runs would be as follows:

$$4 * 4 * 5 = 80$$

Using the Latin Hypercube method has the benefit of needing a fewer number of runs to achieve the same level of confidence than the number required for the Monte Carlo approach because we have guaranteed that the entire probability range will be explored.

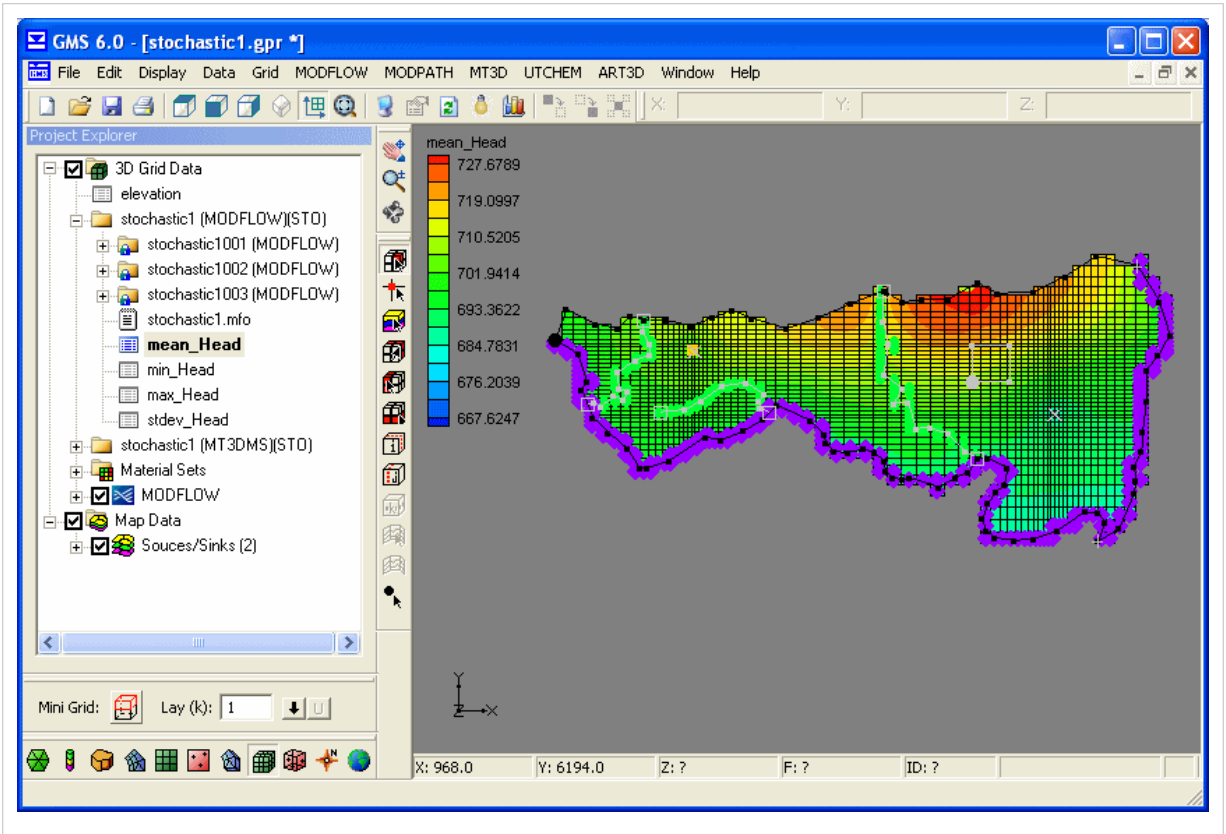
Using Indicator Simulations With Stochastic Modeling

GMS allows you to create a stochastic simulation using output from T-PROGS. This can be in the form of either material sets or HUF data. Use the following steps:

- Generate Material Sets or HUF data using T-PROGS.
- Select the **Stochastic Simulation** from the *Global Options* Dialog.
- Enter the *Stochastic...* dialog from the *MODFLOW* menu.
- Select the Material Sets option and choose the appropriate material set or HUF data simulation.
- Save and Run MODFLOW.
- View the different model results using the Project Explorer.
- Further analyze the results using the Risk Analysis Wizard.
- GMS will generate as many MODFLOW runs as there are material sets.

Statistical Analysis of Stochastic MODFLOW/MT3D solutions

A statistical analysis can be computed on a Stochastic MODFLOW or MT3D solution by right-clicking on a stochastic folder in the Project Explorer and selecting the ***Statistical Analysis*** command. This command creates four data sets for the mean, min, max, and standard deviation. The 3D grid display options can then be used to visualize these data sets.



Gaussian Field Generator

GMS includes an interpolation option associated with the 2D scatter point module called Gaussian Sequential Simulation (GSS). This option is used to generate a set of scalar datasets (Gaussian fields) using a Gaussian sequential simulation. This is somewhat similar to indicator kriging or T-PROGS in that it generates a set of equally probable results which exhibit heterogeneity and are conditioned to values at scatter points. However, the resulting arrays are floating point scalar datasets, rather than the integer arrays produced by T-PROGS and indicator kriging.

The results of a GSS can be used in combination with the new Multiplier Array option for parameters. It is now possible to associate one or more scalar datasets with an array-based parameter. When MODFLOW is executed, the parameter starting value is multiplied by the dataset to produce the input array. This makes it possible to use the results of the Gaussian sequential simulation as input for parameter fields for a stochastic (Monte Carlo) simulation.

Gaussian Simulations

The new GSS tool is based on the FIELDGEN code developed by John Doherty. John Doherty describes GSS as follows:

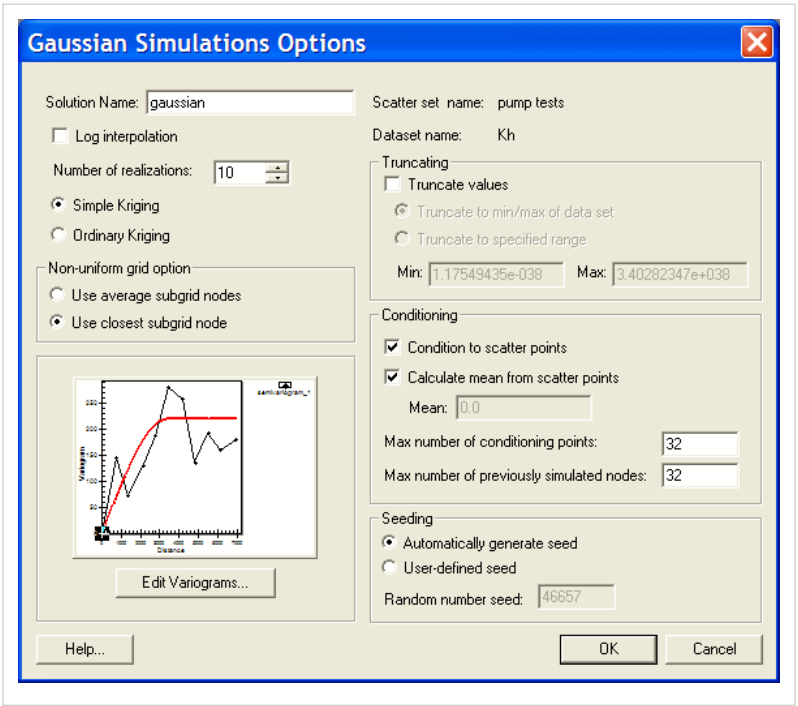
The process of stochastic field generation by sequential simulation is very easy to understand. At each field point an expected field value and a field standard deviation pertaining to that point are first determined. These are calculated through kriging from points to which field values have already been assigned, as well as from points at which conditioning data exists (if available). Using the expected value and standard deviation calculated in this way, a random field value is generated based on the assumption of a Gaussian probability distribution. The field value thus obtained can then be used in generating expected values and standard deviations at other field points at which field generation then takes place in the same way.

GSS is a form of Kriging but it is listed in the GMS interface as a new interpolation scheme. This new option will differ from Kriging in the following ways:

1. GSS uses the FIELDGEN utility developed by John Doherty to perform the interpolation rather than the GSLIB code used by kriging. FIELDGEN is a modified version of the **sgsim** utility in GSLIB so many of the options are quite similar to those used for normal kriging.
2. As is the case with T-PROGS, the user enters the number of desired simulations and FIELDGEN produces N arrays, rather than one array.
3. It can only be used for 2D interpolation and it will only work when interpolating to 3D cell-centered grids.
4. It can work with or without a scatter point set. If a scatter point set is provided, the resulting fields are conditioned to the values at the scatter points. Otherwise the user defines a mean and a variogram and the values are randomly generated.

Gaussian Simulation Options

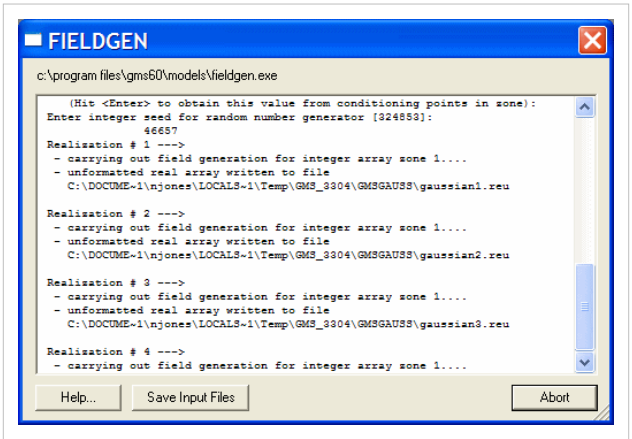
The first step in setting up a GSS is to import a set of scatter points with the values to which you intend to condition your simulation. This step can be skipped if you have no conditioning data. The next step is to select the ***Gaussian Simulation Options*** command in the *Interpolation* menu in the 2D Scatter Point module. This brings up the following dialog:



The **Solution name** at the top is the name that will be applied to the set of Gaussian fields. The **Number of realizations** item is the desired number of Gaussian fields. The original GSLIB code was designed to work with uniform grids (constant cell sizes). The **Non-uniform grid** option controls how the data are converted to a non-uniform grid (if necessary). The **Edit Variogram** button should be selected to set up a model variogram using the GMS variogram editor. A model variogram must be defined whether or not you have scatter points for conditioning.

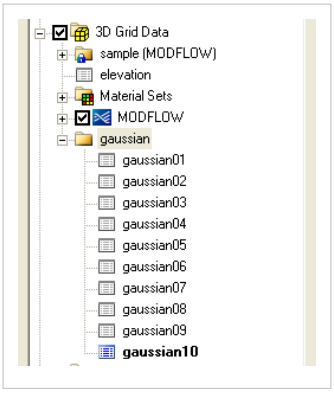
Running the Simulation

Once the GSS options are selected, the next step is to run the simulation. This is accomplished by selecting the ***Run Gaussian Simulation*** command in the *Interpolation* menu. During the simulation, you should see a window displaying the progress of the simulation:

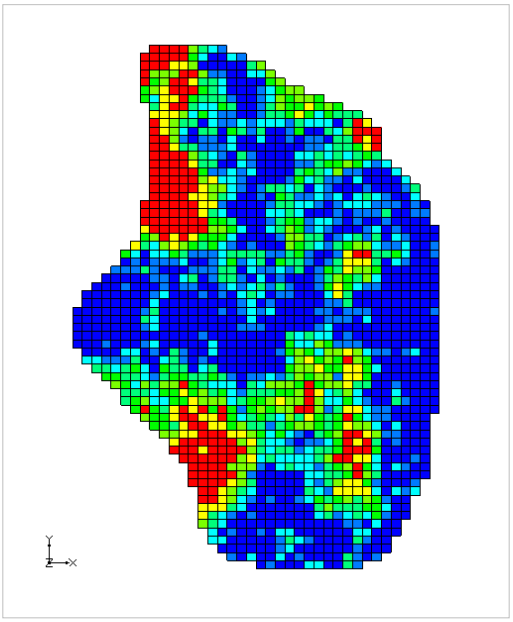


Viewing the Results

Once the simulation is finished, you should see a new folder appear in the Project Explorer window which has the name of the simulation and contains a set of dataset arrays:



Clicking on each dataset icon makes it the active dataset for contouring. The dataset properties can be viewed by double-clicking on the icon. The following image represents a sample Gaussian realization:



Risk Analysis Wizard

The risk analysis wizard is a tool for refining stochastic modeling results. The Risk Analysis Wizard has two options. You can either perform a Capture Zone Analysis or a Threshold Analysis. Capture zone analysis requires a MODFLOW solution set, but threshold analysis can be performed on any solution set type.

Capture Zone Analysis

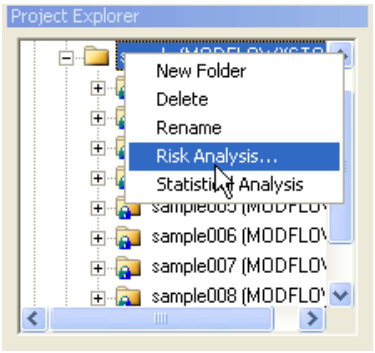
Capture zone analysis includes running MODPATH for each of the MODFLOW solutions to generate a capture zone for each well or zone code group in the MODFLOW model. These capture zones are combined into one probabilistic capture zone

Threshold Analysis

Threshold analysis is similar to capture zone analysis, but threshold analysis can be performed using any type of 3D data set that has been read into the Project Explorer. You first select a simulation set from the Project Explorer. Next, you set up rules for generating a probabilistic threshold dataset. For example, you might be looking at a specific contaminant and want to know what the probability is that the concentration of this contaminant will be above the EPA level for drinking water. You would generate a rule reflecting this limit. After processing all rules for each simulation, GMS creates a probabilistic threshold dataset.

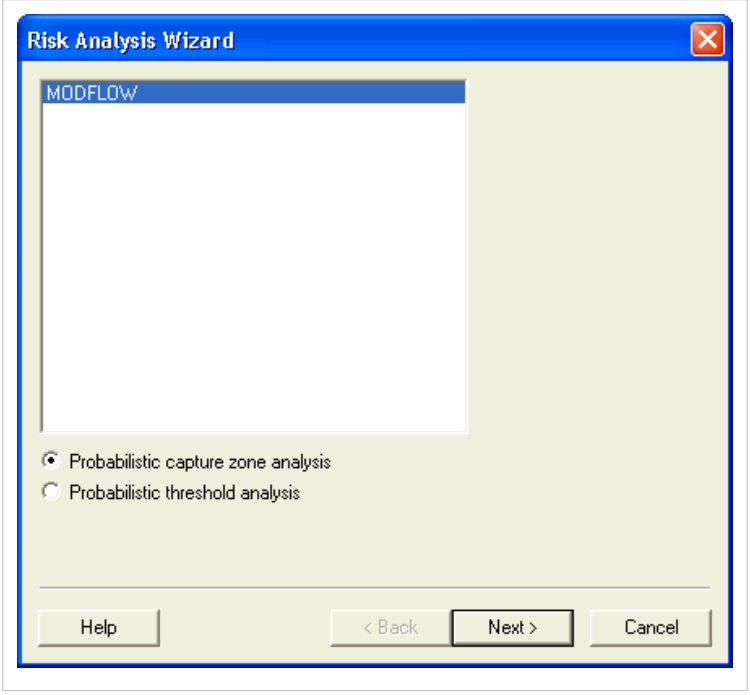
Risk Analysis Wizard Dialogs

The risk analysis wizard is entered through the right-click menu for a folder in the Project Explorer and choose ***Risk Analysis...*** .



Choosing Between Capture Zone and Threshold Analysis

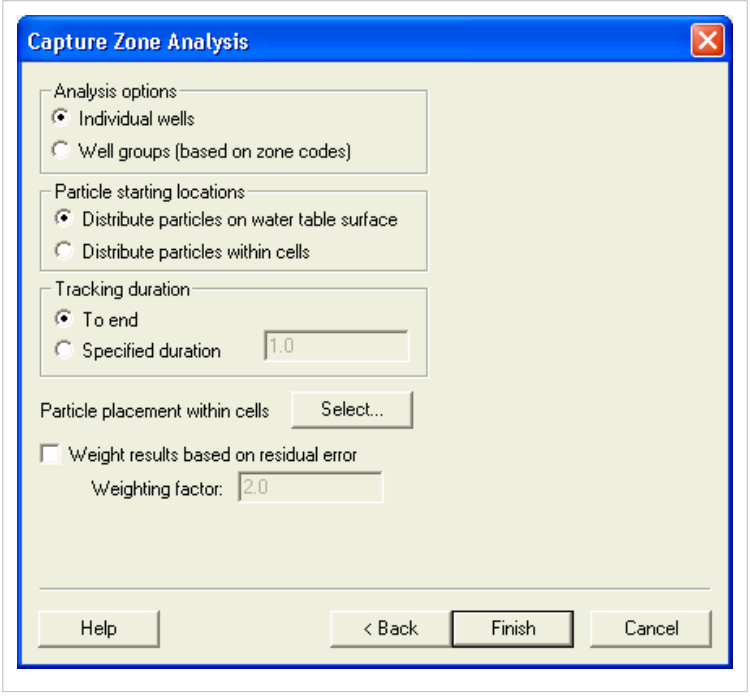
The first step in the risk analysis wizard is to choose what type of simulations you want to process.



The window will list all the solution types as the analysis wizard will only process solutions of the same type. Probabilistic capture zone analysis can only be performed on MODFLOW solutions. Probabilistic threshold analysis can be performed on any solution type.

Capture Zone Analysis Dialog

Capture zone analysis can only be performed on MODFLOW solutions



Analysis Options – Individual wells

Choose this option to create a probabilistic capture zone for each uniquely named well in the MODFLOW model.

Analysis Options – Well groups

Choose this option to create a probabilistic capture zone for each different zone code number.

Particle Starting Locations – Distribute particles on water table surface

Choose this option to distribute particles only on the water table surface. By default, one particle is placed at the *xy* center of the cell at the water table, but you can use the **Particle placement within cells** option to change the number of particles placed on the water table in each cell. This option will create a 2D probabilistic capture zone representing the intersection of the entire 3D probabilistic capture zone with the water table.

Particle Starting Locations - Distribute particles within cells

Choose this option to distribute particles within each cell. By default, one particle is placed at the center of each cell, but you can use the **Particle placement within cells** option to change the number of particles placed on within each cell. This option creates three different probabilistic capture zones. The first represents the 3D capture zone, the other two represent different 2D projections of the 3D capture zone.

Tracking Duration - To end

This option sets MODPATH to move particles through the flow field until they exit the model.

Tracking Duration - Specified duration

This option sets MODPATH to move particles through the flow field until they either exit the model or the time reaches the duration set, which ever comes first.

Particle Placement Within Cells

This option allows you to change the number of particles per cell from the default of one. Increase the number of particles leads to a smoother capture zone, but drastically increases the computation time.

Weight Results Based On Residual Error

In all of the capture zone methods, the algorithms used to synthesize the probability data set can be weighted using observation data. This makes it possible to give more weight to model instances with smaller calibration error when calculating the capture zone probabilities. The weighted head and flow observations can be compared to the computed values to come up with a global error norm, E, for each model run. This error norm can be based on the root mean squared (RMS) error, the sum of the squared weighted residuals, or any other measure selected by the modeler. For capture zone analysis, GMS uses the sum of squared weighted residuals (SSWR) for the error norm. The error norm from each MODFLOW run is used to compute a weight for the given solution using the following equation:

$$w_i = \alpha^{\left[\frac{ME-E_i}{SD}\right]} \quad \text{.....(1)}$$

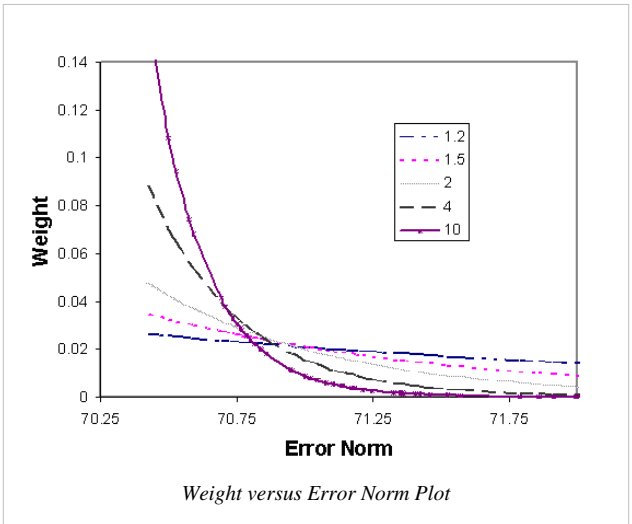
Where W_i is the weight applied to solution i, α is a user-defined factor, ME is the mean of the error values from all solutions, E_{jk} is the error for solution i, and SD is the standard deviation of error values from all solutions. The weights are also normalized as follows

$$w_{final} = \frac{w_i}{\sum w_i} \quad \text{.....(2)}$$

so that the weights sum to unity. Equation 1 was developed to give the greater emphasis to the lower error values and to allow the user to control the relative emphasis given to low vs. high values simply by adjusting the α value. The equation also avoids problems when one of the error values is zero, since a zero error value does not result in an infinite weight. We also wanted the equation to scale the weights according to the data being examined. This is done by subtracting the individual SSWR from the mean error and dividing by the standard deviation.

Equation 1 centers the weights on the mean error. The relative weight given to values differing from the mean is biased by the factor. This makes it possible to bias the resulting weight using knowledge of the site and the quality of the observation data.

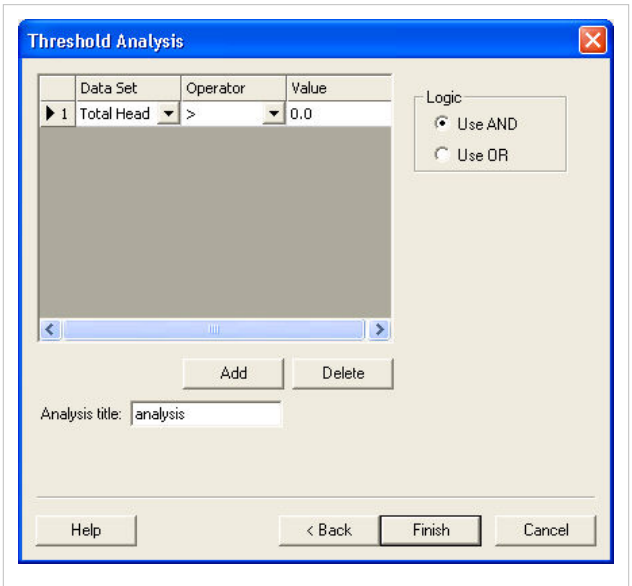
The figure below shows how the α factor in Equation 1 affects the weight applied to a given error. An α factor of 1.2 makes the contribution of each SSWR almost linear, whereas an α factor of ten gives most of the weight to the lowest 5-10 percent while discounting the other error values. We typically use an α value of 2.0.



Weight versus Error Norm Plot

Threshold Analysis Dialog

Threshold analysis can be performed on any collection of 3D datasets. The threshold analysis dataset is created by using rules. For each rule, you select a dataset (only applies to solutions with multiple data sets.), the greater or less than sign and a value. You can have as many rules as you want. The AND and OR logic options allow you to use: 1st rule AND 2nd rule AND 3rd rule; or 1st rule OR 2nd rule OR 3rd rule. Threshold analysis creates one 3D dataset.



Article Sources and Contributors

FEMWATER *Source*: http://www.xmswiki.com/xms/index.php?oldid=30977 *Contributors*: Unjedai

FEMWATER Commands *Source*: http://www.xmswiki.com/xms/index.php?oldid=46298 *Contributors*: Jcreer, Ksmith, Unjedai

Building a FEMWATER Model *Source*: http://www.xmswiki.com/xms/index.php?oldid=59404 *Contributors*: Jcreer, Ksmith

FEMWATER Flows *Source*: http://www.xmswiki.com/xms/index.php?oldid=59420 *Contributors*: Jcreer, Ksmith, Unjedai

Point Source/Sink BC *Source*: http://www.xmswiki.com/xms/index.php?oldid=59413 *Contributors*: Jcreer, Ksmith, Tdye

Assign Node/Face BC *Source*: http://www.xmswiki.com/xms/index.php?oldid=37091 *Contributors*: Jdye, Ksmith

FEMWATER Point / Arc Properties *Source*: http://www.xmswiki.com/xms/index.php?oldid=38736 *Contributors*: Ksmith

FEMWATER Model Input *Source*: http://www.xmswiki.com/xms/index.php?oldid=37095 *Contributors*: Ksmith

FEMWATER Initial Conditions *Source*: http://www.xmswiki.com/xms/index.php?oldid=37096 *Contributors*: Ksmith, Wood

Saving a FEMWATER Simulation *Source*: http://www.xmswiki.com/xms/index.php?oldid=37295 *Contributors*: Jschultze, Ksmith

FEMWATER Display Options *Source*: http://www.xmswiki.com/xms/index.php?oldid=37098 *Contributors*: Ksmith, Tdye

FEMWATER Post Processing Viewing Options *Source*: http://www.xmswiki.com/xms/index.php?oldid=55654 *Contributors*: Jcreer, Ksmith, Unjedai

FEMWATER Particle Sets *Source*: http://www.xmswiki.com/xms/index.php?oldid=33351 *Contributors*: Unjedai

MODAEM *Source*: http://www.xmswiki.com/xms/index.php?oldid=38347 *Contributors*: Djordan, Ksmith, Unjedai

MODAEM License Agreement *Source*: http://www.xmswiki.com/xms/index.php?oldid=30829 *Contributors*: Jdye

MODAEM Display Options *Source*: http://www.xmswiki.com/xms/index.php?oldid=37101 *Contributors*: Ksmith, Wood

MODAEM Commands *Source*: http://www.xmswiki.com/xms/index.php?oldid=46299 *Contributors*: Jcreer, Ksmith, Unjedai

MODFLOW *Source*: http://www.xmswiki.com/xms/index.php?oldid=55724 *Contributors*: Alanlemon, Bdolinar, Htran, Jcreer, Ksmith, Unjedai

MODFLOW-2005 *Source*: http://www.xmswiki.com/xms/index.php?oldid=54486 *Contributors*: Bdolinar, Ksmith, Unjedai

MODFLOW Commands *Source*: http://www.xmswiki.com/xms/index.php?oldid=50078 *Contributors*: Jcreer, Ksmith, Unjedai

MODFLOW Packages Supported in GMS *Source*: http://www.xmswiki.com/xms/index.php?oldid=54505 *Contributors*: Alanlemon, Bdolinar, Ksmith, Unjedai

BCF Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=43966 *Contributors*: Ksmith, Unjedai

CHD Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=35065 *Contributors*: Ksmith

DE4 Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=35692 *Contributors*: Alanlemon, Unjedai

DRN Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=34256 *Contributors*: Ksmith

DRT Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=37105 *Contributors*: Ksmith

ETS Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=37106 *Contributors*: Ksmith

EVT Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=37109 *Contributors*: Ksmith

GHB Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=37110 *Contributors*: Ksmith, Unjedai

Global Options/Basic Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=54494 *Contributors*: Ksmith, Unjedai

GMG Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=36567 *Contributors*: Ksmith, Tdye

HFB Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=37120 *Contributors*: Ksmith

HUF Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=37121 *Contributors*: Ksmith

LAK Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=49944 *Contributors*: Ksmith, Unjedai

LMG Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=37927 *Contributors*: Htran, Ksmith

LMG1 Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=34272 *Contributors*: Ksmith

LPF Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=43967 *Contributors*: Ksmith, Unjedai

MNW1 Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=37125 *Contributors*: Bdolinar, Ksmith

MNW2 Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=37126 *Contributors*: Bdolinar, Ksmith

NWT Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=35929 *Contributors*: Alanlemon, Bdolinar

PCG2 Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=34264 *Contributors*: Ksmith

RCH Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=37127 *Contributors*: Ksmith

PEST ASP Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=37472 *Contributors*: Ksmith, Unjedai

RIV Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=37128 *Contributors*: Ksmith

SIP Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=34262 *Contributors*: Ksmith

SSOR Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=34266 *Contributors*: Ksmith

STR/SFR Packages *Source*: http://www.xmswiki.com/xms/index.php?oldid=52720 *Contributors*: Ksmith, Unjedai

UZF Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=37134 *Contributors*: Htran, Ksmith

WEL Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=37135 *Contributors*: Bdolinar, Ksmith

Building a MODFLOW Model *Source*: http://www.xmswiki.com/xms/index.php?oldid=31689 *Contributors*: Bdolinar

MODFLOW Array Editor *Source*: http://www.xmswiki.com/xms/index.php?oldid=37136 *Contributors*: Ksmith, Wood

MODFLOW Grid Approach *Source*: http://www.xmswiki.com/xms/index.php?oldid=44549 *Contributors*: Alanlemon, Bdolinar, Ksmith

MODFLOW Conceptual Model Approach *Source*: http://www.xmswiki.com/xms/index.php?oldid=50653 *Contributors*: Alanlemon, Ksmith, Unjedai

Activate Cells in Coverage *Source*: http://www.xmswiki.com/xms/index.php?oldid=37142 *Contributors*: Ksmith

Stress Periods *Source*: http://www.xmswiki.com/xms/index.php?oldid=37143 *Contributors*: Ksmith

Map to MODFLOW *Source*: http://www.xmswiki.com/xms/index.php?oldid=50652 *Contributors*: Alanlemon, Ksmith, Unjedai, Wood

Defining the Layer Elevations *Source*: http://www.xmswiki.com/xms/index.php?oldid=37792 *Contributors*: Ksmith

Standard MODFLOW Parameters *Source*: http://www.xmswiki.com/xms/index.php?oldid=55298 *Contributors*: Jcreer, Ksmith

MODFLOW Parameters - Two Methods *Source*: http://www.xmswiki.com/xms/index.php?oldid=31263 *Contributors*: Unjedai

Conductance *Source*: http://www.xmswiki.com/xms/index.php?oldid=50654 *Contributors*: Ksmith, Unjedai

MODFLOW Parameters Disclaimer *Source*: http://www.xmswiki.com/xms/index.php?oldid=31262 *Contributors*: Unjedai

Saving and Reading a MODFLOW Simulation *Source*: http://www.xmswiki.com/xms/index.php?oldid=37171 *Contributors*: Ksmith, Tdye

Output Control *Source*: http://www.xmswiki.com/xms/index.php?oldid=37151 *Contributors*: Ksmith

Importing MODFLOW Files *Source*: http://www.xmswiki.com/xms/index.php?oldid=42193 *Contributors*: Alanlemon, Ksmith, Twood, Wood

MODFLOW with HDF5 *Source*: http://www.xmswiki.com/xms/index.php?oldid=50072 *Contributors*: Bdolinar, Ksmith, Unjedai

Unsupported MODFLOW Features *Source*: http://www.xmswiki.com/xms/index.php?oldid=37162 *Contributors*: Alanlemon, Ksmith

Interpolate to MODFLOW Layers *Source*: http://www.xmswiki.com/xms/index.php?oldid=41264 *Contributors*: Alanlemon, Ksmith

MODFLOW Layers to 2D scatter points *Source*: http://www.xmswiki.com/xms/index.php?oldid=37167 *Contributors*: Ksmith, Unjedai

MODFLOW Source/Sink Dialog *Source*: http://www.xmswiki.com/xms/index.php?oldid=34701 *Contributors*: Ksmith

MODFLOW Display Options *Source*: http://www.xmswiki.com/xms/index.php?oldid=34342 *Contributors*: Ksmith

MODFLOW Post Processing Viewing Options *Source*: http://www.xmswiki.com/xms/index.php?oldid=37800 *Contributors*: Alanlemon, Ksmith, Unjedai

MODFLOW Solution Properties Dialog *Source*: http://www.xmswiki.com/xms/index.php?oldid=35093 *Contributors*: Ksmith

Saving and Reading a MODFLOW Simulation *Source*: http://www.xmswiki.com/xms/index.php?oldid=37171 *Contributors*: Ksmith, Tdye

Cell Properties *Source*: http://www.xmswiki.com/xms/index.php?oldid=59147 *Contributors*: Alanlemon, Jcreer, Ksmith

MODFLOW World File *Source*: http://www.xmswiki.com/xms/index.php?oldid=37173 *Contributors*: Bdolinar, Ksmith, Unjedai

Error Summary Plot *Source*: http://www.xmswiki.com/xms/index.php?oldid=37174 *Contributors*: Ksmith

Zone Budget *Source*: http://www.xmswiki.com/xms/index.php?oldid=36888 *Contributors*: Ksmith, Unjedai, Wood

ZONEBUDGET *Source*: http://www.xmswiki.com/xms/index.php?oldid=36598 *Contributors*: Alanlemon, Ksmith

Viewing Computed Fluxes *Source*: http://www.xmswiki.com/xms/index.php?oldid=37176 *Contributors*: Ksmith, Wood

MODPATH *Source*: http://www.xmswiki.com/xms/index.php?oldid=38331 *Contributors*: Jdye, Morelandtom, Unjedai

MODPATH Particle Tracking *Source*: http://www.xmswiki.com/xms/index.php?oldid=37177 *Contributors*: Ksmith, Tdye, Unjedai

MODPATH Particle Sets *Source*: http://www.xmswiki.com/xms/index.php?oldid=55725 *Contributors*: Jcreer, Ksmith, Unjedai

MODPATH Zone Codes *Source*: http://www.xmswiki.com/xms/index.php?oldid=37179 *Contributors*: Ksmith, Tdye

MODPATH Display Options *Source*: http://www.xmswiki.com/xms/index.php?oldid=37184 *Contributors*: Ksmith, Unjedai, Wood

Exporting Pathlines *Source*: http://www.xmswiki.com/xms/index.php?oldid=43396 *Contributors*: Unjedai

MODPATH Commands *Source*: http://www.xmswiki.com/xms/index.php?oldid=58712 *Contributors*: Jcreer, Ksmith, Unjedai

MT3DMS *Source*: http://www.xmswiki.com/xms/index.php?oldid=44540 *Contributors*: Alanlemon, Ksmith, Unjedai

MT3D Packages *Source*: http://www.xmswiki.com/xms/index.php?oldid=44530 *Contributors*: Alanlemon, Ksmith

MT3D Source/Sink Mixing Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=44539 *Contributors*: Alanlemon, Ksmith

Basic Transport Package Dialog *Source*: http://www.xmswiki.com/xms/index.php?oldid=51688 *Contributors*: Alanlemon, Ksmith, Tdye, Unjedai

ICBUND Array *Source*: http://www.xmswiki.com/xms/index.php?oldid=44535 *Contributors*: Alanlemon, Bdolinar, Ksmith

MT3D Source/Sink Mixing Package *Source*: http://www.xmswiki.com/xms/index.php?oldid=44539 *Contributors*: Alanlemon, Ksmith

MT3D point Sources/Sinks BC *Source*: http://www.xmswiki.com/xms/index.php?oldid=44536 *Contributors*: Alanlemon, Ksmith

Building an MT3DMS Simulation *Source*: http://www.xmswiki.com/xms/index.php?oldid=44533 *Contributors*: Alanlemon, Ksmith

Saving an MT3DMS Simulation *Source*: http://www.xmswiki.com/xms/index.php?oldid=44543 *Contributors*: Alanlemon, Tdye

Importing an MT3D Simulation *Source*: http://www.xmswiki.com/xms/index.php?oldid=37201 *Contributors*: Alanlemon, Ksmith, Unjedai

MT3DMS Display Options *Source*: http://www.xmswiki.com/xms/index.php?oldid=44541 *Contributors*: Alanlemon, Ksmith, Tdye

Calculate Mass *Source*: http://www.xmswiki.com/xms/index.php?oldid=44525 *Contributors*: Alanlemon, Ksmith

MT3D Commands *Source*: http://www.xmswiki.com/xms/index.php?oldid=46302 *Contributors*: Jcreer, Ksmith, Unjedai

PEST *Source*: http://www.xmswiki.com/xms/index.php?oldid=46429 *Contributors*: Alanlemon, Ksmith

PHT3D *Source*: http://www.xmswiki.com/xms/index.php?oldid=47826 *Contributors*: Alanlemon, Jcreer

RT3D *Source*: http://www.xmswiki.com/xms/index.php?oldid=38340 *Contributors*: Jdye, Ksmith, Unjedai

Basic Transport Package Dialog *Source*: http://www.xmswiki.com/xms/index.php?oldid=51688 *Contributors*: Alanlemon, Ksmith, Tdye, Unjedai

SEAM3D *Source*: http://www.xmswiki.com/xms/index.php?oldid=38346 *Contributors*: Jdye, Ksmith, Unjedai

SEAWAT *Source*: http://www.xmswiki.com/xms/index.php?oldid=38695 *Contributors*: Bdolinar, Ksmith

Building a SEAWAT Model *Source*: http://www.xmswiki.com/xms/index.php?oldid=38689 *Contributors*: Bdolinar, Ksmith

SEAWAT Global Options Dialog *Source*: http://www.xmswiki.com/xms/index.php?oldid=38691 *Contributors*: Bdolinar, Ksmith

SEAWAT MODFLOW AUX Variables *Source*: http://www.xmswiki.com/xms/index.php?oldid=38688 *Contributors*: Bdolinar, Ksmith

SEAWAT Packages *Source*: http://www.xmswiki.com/xms/index.php?oldid=38692 *Contributors*: Bdolinar, Ksmith

SEAWAT Importing a SEAWAT Simulation *Source*: http://www.xmswiki.com/xms/index.php?oldid=38696 *Contributors*: Bdolinar, Ksmith

SEAWAT Commands *Source*: http://www.xmswiki.com/xms/index.php?oldid=46303 *Contributors*: Jcreer, Ksmith, Unjedai

SEEP2D *Source*: http://www.xmswiki.com/xms/index.php?oldid=37213 *Contributors*: Ksmith

SEEP2D Display Options *Source*: http://www.xmswiki.com/xms/index.php?oldid=37803 *Contributors*: Ksmith, Tdye

SEEP2D Solution *Source*: http://www.xmswiki.com/xms/index.php?oldid=30366 *Contributors*: Unjedai

SEEP2D Commands *Source*: http://www.xmswiki.com/xms/index.php?oldid=46304 *Contributors*: Jcreer, Ksmith, Unjedai

T-PROGS *Source*: http://www.xmswiki.com/xms/index.php?oldid=52725 *Contributors*: Jcreer, Ksmith, Unjedai, Wood

Vertical Markov Chain *Source*: http://www.xmswiki.com/xms/index.php?oldid=38609 *Contributors*: Ksmith, Unjedai

Strike Dip Markov Chain *Source*: http://www.xmswiki.com/xms/index.php?oldid=39782 *Contributors*: Jcreer, Ksmith

TSIM *Source*: http://www.xmswiki.com/xms/index.php?oldid=55315 *Contributors*: Jcreer, Ksmith, Unjedai

T-PROGS Commands *Source*: http://www.xmswiki.com/xms/index.php?oldid=46305 *Contributors*: Jcreer, Ksmith, Unjedai

TOUGH *Source*: http://www.xmswiki.com/xms/index.php?oldid=55746 *Contributors*: Jcreer, Unjedai

UTEXAS *Source*: http://www.xmswiki.com/xms/index.php?oldid=39699 *Contributors*: Jcreer, Ksmith, Unjedai

UTEXAS Display Options *Source*: http://www.xmswiki.com/xms/index.php?oldid=37224 *Contributors*: Ksmith, Tdye

UTEXAS Commands *Source*: http://www.xmswiki.com/xms/index.php?oldid=46282 *Contributors*: Jcreer, Ksmith, Unjedai

WASH123D Display Options *Source*: http://www.xmswiki.com/xms/index.php?oldid=37225 *Contributors*: Jdye, Ksmith

Model Calibration *Source*: http://www.xmswiki.com/xms/index.php?oldid=55728 *Contributors*: Jcreer, Ksmith

Automated Parameter Estimation *Source*: http://www.xmswiki.com/xms/index.php?oldid=37909 *Contributors*: Alanlemon, Ksmith

Parameter Estimation Dialog *Source*: http://www.xmswiki.com/xms/index.php?oldid=39685 *Contributors*: Jcreer, Ksmith

PEST *Source*: http://www.xmswiki.com/xms/index.php?oldid=46429 *Contributors*: Alanlemon, Ksmith

Run Options *Source*: http://www.xmswiki.com/xms/index.php?oldid=54494 *Contributors*: Ksmith, Unjedai

Observations *Source*: http://www.xmswiki.com/xms/index.php?oldid=37818 *Contributors*: Ksmith, Wood

Plot Wizard *Source*: http://www.xmswiki.com/xms/index.php?oldid=39688 *Contributors*: Bdolinar, Jcreer, Ksmith

Calibration Targets *Source*: http://www.xmswiki.com/xms/index.php?oldid=37240 *Contributors*: Ksmith

Model Checker *Source*: http://www.xmswiki.com/xms/index.php?oldid=37241 *Contributors*: Ksmith, Wood

Parameters *Source*: http://www.xmswiki.com/xms/index.php?oldid=39689 *Contributors*: Jcreer, Ksmith

Parameter Dialog *Source*: http://www.xmswiki.com/xms/index.php?oldid=55294 *Contributors*: Jcreer, Ksmith

Pilot Points *Source*: http://www.xmswiki.com/xms/index.php?oldid=55295 *Contributors*: Jcreer, Ksmith, Wood

Multiplier Arrays for Parameters *Source*: http://www.xmswiki.com/xms/index.php?oldid=55296 *Contributors*: Jcreer, Ksmith

Standard MODFLOW Parameters *Source*: http://www.xmswiki.com/xms/index.php?oldid=55298 *Contributors*: Jcreer, Ksmith

Stochastic Modeling *Source*: http://www.xmswiki.com/xms/index.php?oldid=38615 *Contributors*: Ksmith

Gaussian Field Generator *Source*: http://www.xmswiki.com/xms/index.php?oldid=58981 *Contributors*: Jcreer, Ksmith

Risk Analysis Wizard *Source*: http://www.xmswiki.com/xms/index.php?oldid=39694 *Contributors*: Jcreer, Ksmith

Image Sources, Licenses and Contributors

Image:Topo.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Topo.gif *License*: unknown *Contributors*: Cballard
Image:samp_map.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Samp_map.gif *License*: unknown *Contributors*: Cballard
Image:meshgenc.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Meshgenc.gif *License*: unknown *Contributors*: Cballard
Image:screenlogic.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Screenlogic.gif *License*: unknown *Contributors*: Cballard
Image:time.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Time.gif *License*: unknown *Contributors*: Cballard
Image:3DMeshFolder.GIF *Source*: http://www.xmswiki.com/xms/index.php?title=File:3DMeshFolder.GIF *License*: unknown *Contributors*: Jhandy
Image:dispopts.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Dispopts.gif *License*: unknown *Contributors*: Jdhowlett
Image:MapFolder.GIF *Source*: http://www.xmswiki.com/xms/index.php?title=File:MapFolder.GIF *License*: unknown *Contributors*: Jhandy
Image:Switching_MF2K5.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Switching_MF2K5.jpg *License*: unknown *Contributors*: Bdolinar, Htran
Image:MF2KLPF.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:MF2KLPF.jpg *License*: unknown *Contributors*: Htran
Image:MF2K5LPF.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:MF2K5LPF.jpg *License*: unknown *Contributors*: Htran
Image:changinghead.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Changinghead.gif *License*: unknown *Contributors*: Cballard
Image:drt.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:Drt.png *License*: unknown *Contributors*: Unjedai
Image:Yes_check.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:Yes_check.png *License*: unknown *Contributors*: Unjedai
Image:ofr00-466_1.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:Ofr00-466_1.png *License*: unknown *Contributors*: Unjedai
Image:ets_xy_1.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:Ets_xy_1.png *License*: unknown *Contributors*: Unjedai
Image:ets_xy_2.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:Ets_xy_2.png *License*: unknown *Contributors*: Unjedai
Image:evt.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:Evt.png *License*: unknown *Contributors*: Unjedai
Image:flowbarrier.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Flowbarrier.gif *License*: unknown *Contributors*: Cballard
Image:huf_grid.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Huf_grid.gif *License*: unknown *Contributors*: Cballard
Image:huf_grid_fill.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Huf_grid_fill.gif *License*: unknown *Contributors*: Cballard
Image:lake_bathymetry.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:Lake_bathymetry.png *License*: unknown *Contributors*: Unjedai
Image:mnw.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:Mnw.png *License*: unknown *Contributors*: Unjedai
Image:mnw2.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:Mnw2.png *License*: unknown *Contributors*: Bdolinar
Image:stream.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Stream.gif *License*: unknown *Contributors*: Cballard
Image:Activate1.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Activate1.gif *License*: unknown *Contributors*: Jhandy
Image:tool_insert_row.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Tool_insert_row.gif *License*: unknown *Contributors*: Cballard
Image:tool_remove_row.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Tool_remove_row.gif *License*: unknown *Contributors*: Cballard
Image:maptomodflow1.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Maptomodflow1.jpg *License*: unknown *Contributors*: Ksmith
Image:maptomodflow2.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Maptomodflow2.jpg *License*: unknown *Contributors*: Ksmith
Image:layerele1.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Layerele1.jpg *License*: unknown *Contributors*: Ksmith
Image:layerele2.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Layerele2.jpg *License*: unknown *Contributors*: Ksmith
Image:layerele3.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Layerele3.jpg *License*: unknown *Contributors*: Ksmith
Image:layerele4.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Layerele4.jpg *License*: unknown *Contributors*: Ksmith
Image:layerele5.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Layerele5.jpg *License*: unknown *Contributors*: Ksmith
Image:eq_cond1.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Eq_cond1.gif *License*: unknown *Contributors*: Ksmith, Kwinters
Image:eq_cond2.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Eq_cond2.gif *License*: unknown *Contributors*: Ksmith, Kwinters
Image:eq_cond3.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Eq_cond3.gif *License*: unknown *Contributors*: Ksmith, Kwinters
Image:eq_cond4.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Eq_cond4.gif *License*: unknown *Contributors*: Ksmith, Kwinters
Image:eq_cond5.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Eq_cond5.gif *License*: unknown *Contributors*: Ksmith, Kwinters
Image:eq_cond6.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Eq_cond6.gif *License*: unknown *Contributors*: Ksmith, Kwinters
Image:eq_cond7.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Eq_cond7.gif *License*: unknown *Contributors*: Ksmith, Kwinters
File:Rch.PNG *Source*: http://www.xmswiki.com/xms/index.php?title=File:Rch.PNG *License*: unknown *Contributors*: Htran
File:Chd.PNG *Source*: http://www.xmswiki.com/xms/index.php?title=File:Chd.PNG *License*: unknown *Contributors*: Htran
File:GHB.PNG *Source*: http://www.xmswiki.com/xms/index.php?title=File:GHB.PNG *License*: unknown *Contributors*: Alanlemon
Image:MODFLOWFolder.GIF *Source*: http://www.xmswiki.com/xms/index.php?title=File:MODFLOWFolder.GIF *License*: unknown *Contributors*: Jhandy
image:modflowpostviewing1.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Modflowpostviewing1.jpg *License*: unknown *Contributors*: Ksmith
image:modflowpostviewing2.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Modflowpostviewing2.jpg *License*: unknown *Contributors*: Ksmith
image:modflowpostviewing3.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Modflowpostviewing3.jpg *License*: unknown *Contributors*: Ksmith
Image:ModflowPropertiesDialogBox.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:ModflowPropertiesDialogBox.jpg *License*: unknown *Contributors*: Alanlemon
Image:zone_budget.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Zone_budget.gif *License*: unknown *Contributors*: Cballard
Image:Flow plot.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Flow_plot.jpg *License*: unknown *Contributors*: Cballard
Image:Plot values.JPG *Source*: http://www.xmswiki.com/xms/index.php?title=File:Plot_values.JPG *License*: unknown *Contributors*: Cballard, Unjedai
Image:CCF_datasets.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:CCF_datasets.gif *License*: unknown *Contributors*: Cballard
Image:modpath_pathline_report.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Modpath_pathline_report.gif *License*: unknown *Contributors*: Cballard
Image:3DGridFolder.GIF *Source*: http://www.xmswiki.com/xms/index.php?title=File:3DGridFolder.GIF *License*: unknown *Contributors*: Jhandy
Image:samp_seep.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Samp_seep.gif *License*: unknown *Contributors*: Cballard
Image:flownet1.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Flownet1.gif *License*: unknown *Contributors*: Jhandy
Image:SEEP2D_CM.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:SEEP2D_CM.gif *License*: unknown *Contributors*: Cballard
Image:2DMeshFolder.GIF *Source*: http://www.xmswiki.com/xms/index.php?title=File:2DMeshFolder.GIF *License*: unknown *Contributors*: Jhandy
Image:seep2ddisplay1.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Seep2ddisplay1.jpg *License*: unknown *Contributors*: Ksmith
Image:Matset.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Matset.gif *License*: unknown *Contributors*: Cballard
Image:pathlines.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:Pathlines.png *License*: unknown *Contributors*: Unjedai
Image:markov_graphs.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:Markov_graphs.png *License*: unknown *Contributors*: Unjedai
image:tprogseq1.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Tprogseq1.jpg *License*: unknown *Contributors*: Ksmith
image:tprogseq2.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Tprogseq2.jpg *License*: unknown *Contributors*: Ksmith
Image:rate_matrix.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Rate_matrix.gif *License*: unknown *Contributors*: Cballard
Image:t-progs_wo_boreholes.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:T-progs_wo_boreholes.png *License*: unknown *Contributors*: Unjedai

Image:t-progs_w_boreholes.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:T-progs_w_boreholes.png *License*: unknown *Contributors*: Unjedai
Image:azimuth1.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:Azimuth1.png *License*: unknown *Contributors*: Unjedai
Image:azimuth2.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:Azimuth2.png *License*: unknown *Contributors*: Unjedai
Image:matset_samp.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:Matset_samp.png *License*: unknown *Contributors*: Unjedai
Image:huf_sample.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Huf_sample.gif *License*: unknown *Contributors*: Cballard
Image:markov_chains_z.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:Markov_chains_z.png *License*: unknown *Contributors*: Unjedai
Image:markov_chain_plot.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:Markov_chain_plot.png *License*: unknown *Contributors*: Unjedai
Image:gameas.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:Gameas.png *License*: unknown *Contributors*: Unjedai
Image:verticalchain2.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Verticalchain2.jpg *License*: unknown *Contributors*: Ksmith
Image:verticalchain3.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Verticalchain3.jpg *License*: unknown *Contributors*: Ksmith
Image:markov_chains_x.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:Markov_chains_x.png *License*: unknown *Contributors*: Unjedai
Image:strikedipchain1.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Strikedipchain1.jpg *License*: unknown *Contributors*: Ksmith
Image:UtexasGmsScreenShot.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:UtexasGmsScreenShot.png *License*: unknown *Contributors*: Unjedai
Image:ProfileLinesExampleB.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:ProfileLinesExampleB.png *License*: unknown *Contributors*: Unjedai
Image:ProfileLinesExampleA.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:ProfileLinesExampleA.png *License*: unknown *Contributors*: Unjedai
Image:UTEXASTreeModelIcon.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:UTEXASTreeModelIcon.png *License*: unknown *Contributors*: Unjedai
Image:UtexasHeadDisplayOption.png *Source*: http://www.xmswiki.com/xms/index.php?title=File:UtexasHeadDisplayOption.png *License*: unknown *Contributors*: Unjedai
Image:calib_plot.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Calib_plot.jpg *License*: unknown *Contributors*: Cballard
Image:observeq1.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Observeq1.jpg *License*: unknown *Contributors*: Ksmith
Image:observeq2.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Observeq2.jpg *License*: unknown *Contributors*: Ksmith
Image:comp_v_obs_plot.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Comp_v_obs_plot.gif *License*: unknown *Contributors*: Cballard
Image:comp_v_obs_wt_plot.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Comp_v_obs_wt_plot.gif *License*: unknown *Contributors*: Cballard
Image:res_v_obs_plot.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Res_v_obs_plot.gif *License*: unknown *Contributors*: Cballard
Image:res_v_obs_wt_plot.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Res_v_obs_wt_plot.gif *License*: unknown *Contributors*: Cballard
Image:par_sen_plot.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Par_sen_plot.gif *License*: unknown *Contributors*: Cballard
Image:error_v_sim_plot.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Error_v_sim_plot.gif *License*: unknown *Contributors*: Cballard
Image:error_v_time_plot.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Error_v_time_plot.gif *License*: unknown *Contributors*: Cballard
Image:err_summary_plot.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Err_summary_plot.gif *License*: unknown *Contributors*: Cballard
Image:time_series_plot.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Time_series_plot.gif *License*: unknown *Contributors*: Cballard
Image:active_data_time_series_plot.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Active_data_time_series_plot.gif *License*: unknown *Contributors*: Cballard
Image:flowbudgetplot.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Flowbudgetplot.gif *License*: unknown *Contributors*: Cballard
Image:Calibtarget1.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Calibtarget1.gif *License*: unknown *Contributors*: Jhandy
Image:zonation.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Zonation.gif *License*: unknown *Contributors*: Cballard
Image:Pilot_Point_Cond.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Pilot_Point_Cond.gif *License*: unknown *Contributors*: Cballard
Image:multiplier_array_param_dialog.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Multiplier_array_param_dialog.gif *License*: unknown *Contributors*: Cballard
Image:stochasticeq1.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Stochasticeq1.jpg *License*: unknown *Contributors*: Ksmith
Image:stochasticeq2.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Stochasticeq2.jpg *License*: unknown *Contributors*: Ksmith
Image:freq.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Freq.gif *License*: unknown *Contributors*: Cballard
Image:stochasticeq3.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Stochasticeq3.jpg *License*: unknown *Contributors*: Ksmith
Image:stochasticeq4.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Stochasticeq4.jpg *License*: unknown *Contributors*: Ksmith
Image:StatAnalysis.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:StatAnalysis.gif *License*: unknown *Contributors*: Kwinters
Image:gaussian_sim_options.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Gaussian_sim_options.gif *License*: unknown *Contributors*: Cballard
Image:gaussian_fieldgen_wrapper.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Gaussian_fieldgen_wrapper.gif *License*: unknown *Contributors*: Cballard
Image:gaussian_sim_results.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Gaussian_sim_results.gif *License*: unknown *Contributors*: Cballard
Image:image06.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Image06.gif *License*: unknown *Contributors*: Cballard
Image:Tree_Risk_Anaylsis.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Tree_Risk_Anaylsis.gif *License*: unknown *Contributors*: Cballard
Image:ra_3.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Ra_3.gif *License*: unknown *Contributors*: Cballard
Image:ra_4.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Ra_4.gif *License*: unknown *Contributors*: Cballard
Image:riskwizardeq1.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Riskwizardeq1.jpg *License*: unknown *Contributors*: Ksmith
Image:alpha_char.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Alpha_char.gif *License*: unknown *Contributors*: Cballard
Image:riskwizardeq2.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Riskwizardeq2.jpg *License*: unknown *Contributors*: Ksmith
Image:wt_plot1.gif *Source*: http://www.xmswiki.com/xms/index.php?title=File:Wt_plot1.gif *License*: unknown *Contributors*: Jhandy
Image:ra_1.jpg *Source*: http://www.xmswiki.com/xms/index.php?title=File:Ra_1.jpg *License*: unknown *Contributors*: Cballard