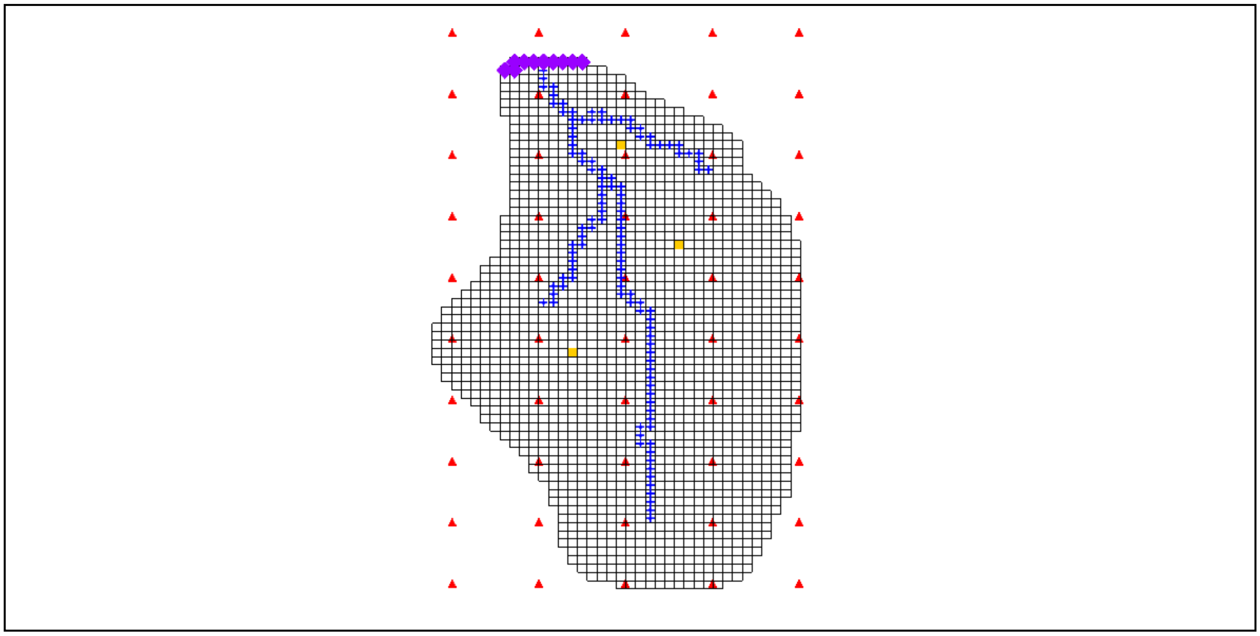
GMS 10.0 Tutorial

MODFLOW – PEST Pilot Points

Use pilot points with PEST to automatically calibrate a MODFLOW model



Objectives

Learn the features and options related to pilot points when used with PEST. Use fixed value pilot points, regularization, and multiple parameters.

Prerequisite Tutorials

- MODFLOW – Automated Parameter Estimation

Required Components

- Grid Module
- Geostatistics
- Map Module
- MODFLOW
- Inverse Modeling

Time

- 45-65 minutes

1 Introduction

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. Using pilot points, values will vary from cell to cell. When the inverse model runs, the values at the pilot points are adjusted and reinterpolated to the grid cells until the objective function is minimized.

PEST provides an option for the pilot point method called regularization. Regularization imposes an additional measure of “stiffness” to the parameter being interpolated. This “stiffness” is imposed by providing PEST with additional information about the parameter in the form of prior information equations. 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.

There are two methods available in GMS for defining the prior information equations for PEST. The two methods can be used simultaneously but usually they are used separately.

The first method is **Preferred homogeneous regularization**. When this option is selected the prior information equations written to the PEST control file relate the pilot points to one another. These equations indicate to PEST that in the absence of any strong influence from the PEST objective function, pilot points that are near to one another should have about the same value.

The second method of regularization available in GMS is preferred value regularization. When this option is selected, prior information equations written to the PEST control file relate the pilot points to their starting value. These equations indicate to PEST that, in the absence of any strong influence from the PEST objective function, the pilot point values should be equal to their starting value. Depending on the particular problem that the user is trying to solve, one method may be preferable over the other.

1.1 Outline

Here are the steps of the tutorial:

1. Open a MODFLOW model and solution.
2. Create pilot points and run PEST.
3. Load optimal parameter values and view the resulting HK field.
4. Include pilot points with fixed values and run PEST.
5. Change regularization options and run PEST.
6. Use pilot points on different zones and different parameter types.

2 Description of Problem

The model to be calibrated in this tutorial is the same model featured in the "MODFLOW – Model Calibration" tutorial. The model includes observed flow data for the stream and observed heads at a set of scattered observation wells. The conceptual model for the site consists of a set of recharge and hydraulic conductivity zones. These zones will be marked as parameters and an inverse model will be used to find a set of recharge and hydraulic conductivity values that minimize the calibration error.

3 Getting Started

Do the following to get started:

1. If necessary, launch GMS.
2. If GMS is already running, select the *File* | **New** command to ensure that the program settings are restored to their default state.

4 Reading in the Project

First, read in the modeling project:

1. Select the **Open** button.
2. Locate and open the *Tutorials\MODFLOW\pilotpoints* directory.
3. Select the file entitled “start.gpr.”
4. Click the **Open** button.
5. Expand the “Map Data” folder and the “BigVal” conceptual model.

The user should see a MODFLOW model with a solution and a set of map coverages. Three of the coverages are the source/sink, recharge, and hydraulic conductivity coverages used to define the conceptual model. The active coverage contains a set of observed head values from observation wells. If the user switches to the source/sink coverage, he or she will notice that an observed flow value has been assigned to the stream network.

This model has already been parameterized, so the user just needs to create the pilot points and then run PEST.

5 Creating Pilot Points

The user will create the pilot points that define the hydraulic conductivity distribution for the model. The pilot points are defined as 2D scatter point sets in GMS. It should be noted that there are many different ways in GMS to create 2D scatter points. Scatter points can be created by converting a 2D Grid, 2D Mesh, TIN, Borehole contacts, or Map data to a scatter point set. The easiest way to create scatter points is to create a new scatter point set and then click out the points in the graphics window.

In this example, the user will create a 2D grid and then convert it to scatter points. It is necessary to create about 50 pilot points in order to make a cell-centered 2D Grid with 50 cells.

1. In the Project Explorer, right-click on the empty space.
2. From the pop-up menu, select the *New* | **Grid Frame** command.
3. In the Project Explorer, right-click on the *Grid Frame* .
4. Select the **Fit to Active Coverage** command.
5. If necessary, resize the grid frame with the **Grid Frame** tool if the grid frame doesn’t encompass the entire model.

Now that the coverages and the Grid Frame are created, it is now possible to create the grid.

6. Select the Feature Objects | **Map → 2D Grid** command to open the *Create Finite Difference Grid*.
7. Enter “5” for the *Number Cells in the X-Dimension*.
8. Enter “10” for the *Number Cells in the Y-Direction*.
9. Select the **OK** button.

The result is a 2D grid with 50 cells. The user can convert it to 2D Scatter Points like so:

10. Right-click on the “grid” item under the “2D Grid Data” folder.
11. Select the *Convert to* **| 2D Scatter Points** command.
12. Enter “HK” for the name of the new scatter set.
13. Select *OK*.
14. Right-click on the “grid” again.
15. Select the **Delete** command.

The default starting value of hydraulic conductivity should be 0.5 m/d, so the user will change the data values at the scatter points to this value.

16. If necessary, expand the “2D Scatter Data” folder in the Project Explorer.
17. Select the “HK” scatter point set from the Project Explorer.
18. Unlock the scatter points by selecting the *Scatter Points* | **Lock All Scatter Points** menu command.
19. Select the **Select Scatter Points** tool.
20. Type CTRL+A to select all the points (or click the *Edit* | Select All menu command).
21. In the *Edit XYZF* toolbar, for the *F value*, enter “0.5.”
22. Hit *Enter*.
23. Then deselect the points by clicking anywhere outside the model.

The graphics window should look similar to the following figure.

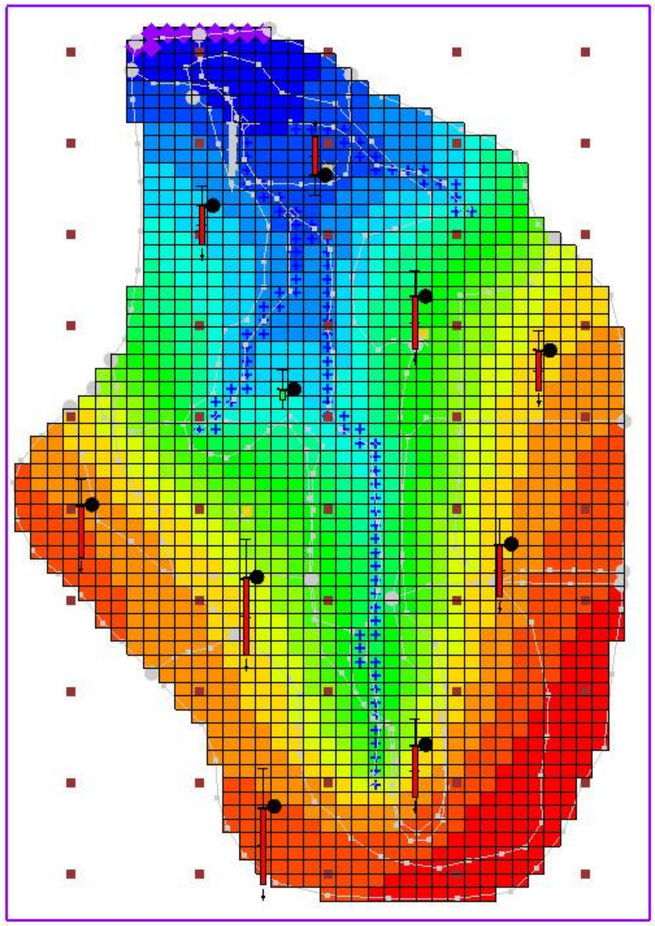


Figure 1 Placement of scatter points

6 Editing the HK parameter

In the "MODFLOW – Automated Parameter Estimation" example, the tutorial had four hydraulic conductivity parameters. For this problem, the user is estimating the hydraulic conductivity for the entire layer with the pilot points. Therefore, the user only needs one parameter for hydraulic conductivity. This parameter will then be linked to the pilot points using the *Parameters* dialog.

6.1 Editing the Parameters

Now edit the currently defined parameters for MODFLOW.

1. Select the *MODFLOW* | **Parameters** command to open the *Parameters* dialog.
2. For parameter "HK_30," select the drop down arrow in the *Value* column.

3. Then select "<Pilot points>" from the drop down list.

The interpolation options associated with the pilot points can be changed by clicking on the small button above the drop down arrow in the *Value* column.

4. Click on the button above the drop down arrow in the *Value* column for parameter *HK_30*.

This brings up the *2D Interpolation Options* dialog. Here, the user can select the scatter point set and dataset used with the parameter as well as the interpolation scheme.

5. The defaults are appropriate in this case, so it's not necessary to change anything.
6. Select **OK** to exit the *2D Interpolation Options* dialog.
7. Select **OK** to exit the *Parameters* dialog.

6.2 Limiting the Number of Parameter Estimation Runs

In the interest of time, this tutorial will limit the number of iterations that PEST does for the problem.

1. Select the *MODFLOW* | **Parameter Estimation** command.
2. Change the *Max number of iterations (NOPTMAX)* to "5."

Notice the *Tikhonov regularization* section of the dialog. In this section, the user can specify the type of regularization to use with PEST. By default, *Preferred homogeneous regularization* is turned on.

The *Prior information power factor* is used to change the weight applied to the prior information equations for the pilot points. 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.

3. Select **OK** to exit the dialog.

7 Saving the Project and Running PEST

Now save and run PEST.

1. Select the *File* | **Save As** command.

2. Change the project name to "mfpest_pilot.gpr."

3. Click the **Save** button.

4. Select the **Run MODFLOW** button.

PEST is now running. The error and parameter values are shown in the spreadsheet in the upper right side of the dialog and the plot on the left shows the error. In this case, the user may notice some strange parameter names like sc1v1. These names were automatically generated and assigned to the pilot points.

PEST will take several minutes to run. The user should see the residual error decrease. When PEST is finished, a message will appear in the text portion of the window and the **Abort** button will change to **Close**.

8 Viewing the Solution

Once PEST is finished, it is possible to read in the solution.

1. Make sure that the *Read solution on exit* toggle is checked.

2. Select the **Close** button.

The contours currently shown on the 3D grid are the heads from the MODFLOW run with the optimum parameter values. The user will now look at the observation targets in the map model and the error associated with this model run.

3. In the Project Explorer, turn off the "3D Grid Data" folder in order to see the coverage data better.

4. Expand the "BigVal" conceptual model.

5. Select the "Sources & Sinks" coverage from the Project Explorer. Notice that the observation target on the arc group almost exactly matches.

6. Select the **Select Arc Group** tool.

7. Select the arc group by clicking on the river arc. Notice in the edit strip at the bottom of the graphics window the computed and observed flow is reported.

8. Select the "Observation Wells" coverage from the Project Explorer to see how closely the computed heads match the field observations.

9. If necessary, expand the "3d Grid Data" folder and the "grid" item.

10. Right-click on the "mfpest_pilot (MODFLOW)" solution in the Project Explorer.

11. Select the **Properties** command to open the *Properties* dialog.

This command brings up a spreadsheet showing the error from this model run. The spreadsheet shows the error from the head observations, the flow observations, and the combined weighted observations. Note that these values are lower than the values obtained using the zonal parameters approach.

12. When finished viewing the properties, select **Done**.

9 Viewing the Final Hydraulic Conductivity

When PEST ran a new conductivity, value was estimated at each of the scatter points used with the “HK_30” parameter. Now the user will read in the optimal parameter values as determined by PEST. Reading in the optimal parameter values will create a new dataset for the scatter point set. Then the user can see the final hydraulic conductivity field.

1. In the Project Explorer, turn on the “3D Grid Data” folder.
2. Select the *MODFLOW* | **Parameters** command to open the *Parameters* dialog.
3. Click the **Import Optimal Values** button.
4. Go to the *Tutorials\MODFLOW\pilotpoints\mfpest_pilot_MODFLOW* directory.
5. Select the “mfpest_pilot.par” file and select the *Open* button. Notice that the starting values for the parameters have changed.
6. View the pilot point options by selecting the button above the drop down arrow in the *Value* column for parameter “HK_30.”

The *2D Interpolation Options* dialog will appear. Notice the “HK_30 (mfpest_pilot)” dataset is listed as the one being used by the pilot points. This dataset was imported when the user imported the optimal values and represents the optimal values at each pilot point as determined by PEST.

7. Select OK to exit the *2D Interpolation Options* dialog.
8. Select OK to exit the *Parameters* dialog.
9. Expand the “MODFLOW” item in the Project Explorer.
10. Under the “LPF” package, select the “HK” dataset.

The user should now see the final hydraulic conductivity values for the MODFLOW simulation.

10 Adding Fixed Value Pilot Points

Pilot points can be supplemented by field measured hydraulic conductivity values (such as pump test data values). The user will now add additional pilot points to the model and fix the HK value at those points. First, it is necessary to change the display so it is possible to see the grid.

1. Select the **Display Options** button.
2. Turn off the *Contours* option.
3. Select **OK**.

Notice that there are 3 pumping wells in the model. For purposes of illustration, the user will assume that a pump test was performed at each of these wells and that the HK was estimated. The user will create a pilot point at each of these wells.

4. Select the "2D Scatter Data" folder in the Project Explorer.
5. Select the **Create Scatter Points** tool.
6. Create a scatter point at each of the pumping wells as shown in the following figure.

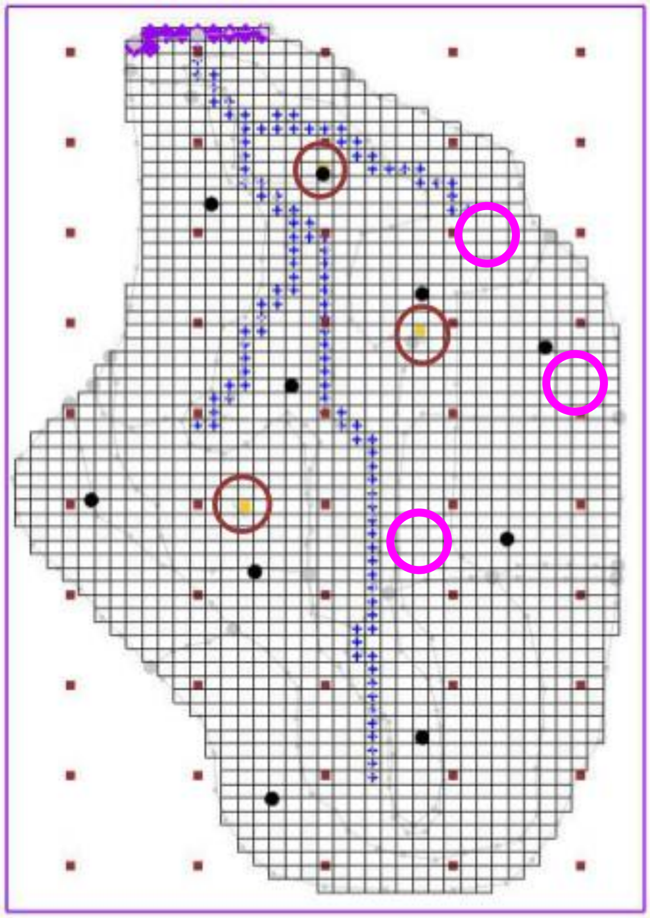


Figure 2. Location of pumping wells.

7. Make sure the *Scatter Points* | **Lock All Scatter Points** menu command is not checked.

8. Select the **Select Scatter Points** tool.

9. Select the new scatter point for the well closest to the top of the model. The user may want to turn off the 3D Grid in the Project Explorer to more easily see the new scatter points.

10. In the *F:* field near the top of the GMS window, enter "1.0."

11. Now, select the scatter point at the well on the east (right) side of the model and enter **0.1 in** the *F:* field.

12. Next, select the scatter point at the well on the west (left) side of the model and enter "5.0" in the *F:* field.

13. Finally, select all three of the new scatter points (hold the shift key down to multiselect).

14. Then select the *Edit* | **Properties** command to open the *Properties* dialog.

15. Toggle on the *Fixed Pilot Point* field for each of the points.
16. Select **OK**.

11 Saving the Project and Running PEST

It is now possible to save and run PEST.

1. Select the *File* | **Save As** command.
2. Change the project name to **“**mfpest_pilot_fixed.gpr.”
3. Click the **Save** button.
4. Select the **Run MODFLOW** button.

PEST will take several minutes to run. Once PEST is finished, the user can read in the solution.

5. Make sure that the *Read solution on exit* toggle is checked.
6. Select the **Close** button.

The user may wish to view the new HK field by importing the optimal values and examining the contours as was done previously.

12 Changing the Regularization Option

The user will now change the regularization option to use the *Preferred value regularization* method.

1. Select the *MODFLOW* | **Parameter Estimation** command to open the *PEST* dialog.
2. Turn off the *Preferred homogeneous regularization* toggle.
3. Turn on the *Preferred value regularization* toggle.
4. Select *OK*.

13 Saving the Project

Now save the project.

1. Select the *File* | **Save As** command.
2. Change the project name to **“**mfpest_pilot_pref_val.gpr.”

3. Click the **Save** button.

13.1 Prior Information equations

The user can compare the different prior information equations written from GMS by looking at the RPF files in the MODFLOW directories. The prior information equations for *Preferred homogenous regularization*, found in mfpest_pilot.rpf should look like the following:

```
pi0 1.0 * log(sc1v1) - 1.0 * log(sc1v2) = 0.0 0.0018556829581 regul_1
pi1 1.0 * log(sc1v1) - 1.0 * log(sc1v3) = 0.0 0.0003314571401 regul_1
pi2 1.0 * log(sc1v1) - 1.0 * log(sc1v4) = 0.0 0.0000983152822 regul_1
```

Notice that these equations define a relationship between the different pilot points. In addition, the weight applied to theses equations changes as shown by the last number written to each line. In contrast, the prior information equations for *Preferred value regularization*, found in mfpest_pilot_pref_val.rpf shown below, have the same weight applied and define a preferred value for each point.

```
pi0 1.0 * log(sc1v1) = -0.877359449863 1.0 regul_1
pi1 1.0 * log(sc1v2) = -0.87738275528 1.0 regul_1
pi2 1.0 * log(sc1v3) = -0.764383137226 1.0 regul_1
```

14 Running PEST

Now run PEST.

1. Select the **Run MODFLOW** button.

PEST will take several minutes to run. Once PEST is finished, the user can read in the solution.

2. Make sure that the *Read solution on exit* toggle is checked.

3. Select the **Close** button.

The user may wish to view the new HK field by importing the optimal values and examining the contours as was done previously.

15 Multiple Parameters using Pilot Points

In GMS, pilot points can be used with HK and RCH parameters. Also, the user can have multiple HK (or RCH) parameters that use the same or different pilot points. The user will now create a second HK parameter and create a new set of pilot points.

1. In the Project Explorer, turn off the 3D grid.

2. Select the "Hydraulic Conductivity" coverage from the Project Explorer.

3. Select the **Select Polygons** tool, and double-click the polygon surrounding the river in the middle of the model.

4. In the *Attribute Table* dialog, enter a value of "-60.0" for the *Horizontal K* and select *OK*.

5. Right-click on the "Hydraulic Conductivity" coverage and select the *Map To* | **MODFLOW/MODPATH** command.

15.1 Creating a Second Set of Pilot Points

Now the user will create another scatter point set for the new HK parameter. The user will again create a 2D grid and convert it to a scatter point set.

1. In the Project Explorer, right-click on the empty space.

2. From the pop-up menu, select the *New* | **2D Grid** command to open the *Create Finite Difference Grid* dialog.

3. Enter the values shown in the following figure to create the 2D Grid.

4. Make sure to enter "0.5" for the Origin in the Z-Dimension section as this will be the value assigned to the scatter points created from the grid.

5. Also, make sure that the *Grid type* near the bottom of the dialog is set to *Cell centered*.

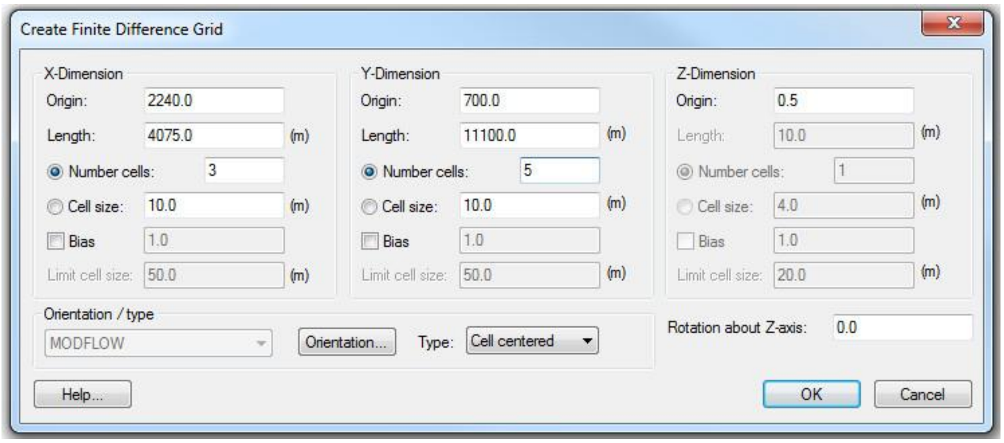


Figure 3 Create 2D Grid dialog

6. When finished entering the values, click **OK.**

7. Right-click on the "grid" under the "2D Grid Data" folder.

8. Select the *Convert to* | **2D Scatter Points** command.

9. Enter "HK_60" for the name of the new scatter set.

10. Right-click on the same "grid" item.

11. Select the **Delete** command

15.2 Creating the New HK Parameter

Now create a new parameter for the newly created pilot points.

1. Select the *MODFLOW* | **Parameters** command to open the *Parameters* dialog.
2. Select the **Initialize From Model** button.
3. If necessary, turn on the toggles in the *Param. Est. Solve* column and the *Log Xform* column for the “HK_60” parameter.
4. Select the drop down arrow in the *Value* column for the “HK_60” parameter.
5. Then select “<Pilot points>” from the drop down list.
6. Click on the button above the drop down arrow in the *Value* column for parameter “HK_60.” This will open the *2D interpolation Options* dialog.
7. Make sure that the scatter point set selected in the dialog is “HK_60 (active).”
8. Select **OK** to exit the *2D interpolation Options* dialog.
9. Select **OK** to exit the *Parameters* dialog.

15.3 Using Pilot Points with RCH Parameter

The user will also use pilot points to estimate recharge with the model. For the RCH parameter, the user will use the same set of pilot points that the HK_30 parameter uses, but the user will create a new dataset with starting values for the RCH parameter.

1. Right-click the “Recharge” coverage from the Project Explorer.
2. Select the **Attribute Table** command.
3. Change the *Feature type* to “Polygons” at the top of the dialog.
4. In the *All* row, change the value of *Recharge rate* to “-150.0.”
5. Select *OK*.
6. Right-click on the “Recharge” coverage and select the *Map To* | **MODFLOW/MODPATH** command.

Creating New Starting Values for the RCH Parameter

Now create a new dataset on the HK scatter set to provide the starting values for the RCH parameter.

7. Select the “HK” scatter point set from the Project Explorer.

8. Select the *Edit* | **Dataset Calculator** command.

9. Enter “1e-5” in the *Expression* field.

10. Enter “RCH” in the *Result* field.

11. Select the **Compute** button to create a new dataset with all values equal to “1.0e-5.”

12. Select **Done** to exit the dialog.

Editing the RCH Parameters

Now edit the RCH parameters to use pilot points.

1. Select the *MODFLOW* | *Parameters* command.

2. Delete the **RCH_180** and **RCH_210** parameters by selecting the row and then the *Delete* button.

3. Turn on the *Pilot Points* option for parameter **RCH_150** by selecting the drop down arrow in the *Value* column. Then select **<Pilot points>** from the drop down list.

4. Click on the button above the drop down arrow in the *Value* column for parameter **RCH_150**. Make sure that the scatter point set selected in the dialog is **HK** and that the dataset is **RCH**.

5. Select *OK* twice to exit both dialogs.

16 Saving the Project and Running PEST

Now save and run PEST.

1. Select the *File* | **Save As** command.

2. Change the project name to **“**mfpest_pilot_2zones.gpr.”

3. Click the **Save** button.

When pilot points are assigned to both HK and RCH parameters, the prior information equations for the HK and RCH parameters are assigned to different regularization groups. According to John Doherty, this helps PEST to differentiate weighting amongst pertinent prior information equations (read as: PEST works better with this option).

4. Select the **Run MODFLOW** button.

PEST will take several minutes to run. Once PEST is finished, the user can read in the solution.

5. Make sure that the *Read solution on exit* toggle is checked. Select the **Close** button.

The user may wish to view the new HK field by importing the optimal values and examining the contours as was done previously.

17 A Note on Highly Parameterized Models

The model that was just created has over 100 parameters. This is a fairly simple MODFLOW model that converges rather quickly; most real world problems take longer to run. Thus, it may not be practical to run MODFLOW over 100 times for each PEST iteration. However, PEST supports a very innovative method known as SVD-Assist which can dramatically reduce the number of model runs required for each PEST iteration. When the user combines SVD-Assist with Parallel PEST, it becomes practical to use PEST with models containing hundreds or even thousands of parameters. The user can learn more about these methods in the tutorial: "MODFLOW – Advanced PEST."

18 Conclusion

This concludes the "MODFLOW – PEST Pilot Points" tutorial. Here are the key concepts in this tutorial:

- When using pilot points, the user may have more parameters than observations because regularization is included in the parameter estimation.
- In the *MODFLOW Parameters* dialog, the user can change a parameter to use pilot points by using the button.
- 2D scatter points can be used to create pilot points in GMS.

