

v. 10.3

GMS 10.3 Tutorial **MODFLOW-USG – PEST**

Model calibration with PEST



Objectives

Learn how to calibrate a MODFLOW-USG model using PEST.

Prerequisite Tutorials

- MODFLOW Model Calibration
- MODFLOW Automated Parameter Estimation

Required Components

- Grid Module
- Map Module
- MODFLOW
- Inverse Modeling

Time

• 25–40 minutes



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1 Introduction

The "MODFLOW – Automated Parameter Estimation" tutorial should be completed prior to beginning this tutorial. This tutorial discusses and demonstrates opening a MODFLOW model and solution, converting it to a MODFLOW-USG model, running PEST, and loading optimal parameter values.

1.1 Getting Started

Do the following to get started:

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

1.2 Importing the Project

First, import the modeling project:

- 1. Click **Open** \overrightarrow{D} to bring up the *Open* dialog.
- 2. Select "Project Files (*.gpr)" from the *Files of type* drop-down.
- 3. Browse to the *Tutorials\MODFLOW-USG\UsgPest* directory and select "mf2k_pest_zones.gpr".
- 4. Click **Open** to import the project and exit the *Open* dialog.

The imported project should appear similar to Figure 1.



Figure 1 Initial screen after importing the project

Notice there is now a MODFLOW model with a solution and a set of map coverages (Figure 2). 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.

Feel free to switch to the "O Sources & Sinks" coverage and use the **Select Arc Group** f tool to select the stream network. This makes the observed flow value visible in the status bar. Switch back to the "O Observation Wells" coverage when done.



Figure 2 Initial appearance of the Project Explorer

2 Converting to a MODFLOW-USG Model

The existing model is a MODFLOW-2000 model. This will be converted to a MODFLOW-USG model before running PEST.

- 1. Right-click on" MODFLOW" in the Project Explorer and select **Convert to MODFLOW-USG Simulation...** to bring up a prompt asking to include inactive cells in the new UGrid.
- 2. Click **No** to close the prompt.
- 3. Click **OK** to acknowledge that the PCG package is not supported by MODFLOW-USG.
- 4. Right-click on the " I 3D Grid Data" folder in the Project Explorer and select the **Delete** to remove the 3D grid from the project.

The model should now appear similar to Figure 3.



Figure 3 Model after conversion to MODFLOW-USG

2.1 Saving and Running MODFLOW-USG

Next, save the project and run MODFLOW-USG.

1. Select *File* | **Save As...** to bring up the *Save As* dialog.

- 2. Enter "mfusg_pest.gpr" as the *File name*.
- 3. Click **Save** to save the project under the new name and close the *Save As* dialog.
- 4. Click **Run MODFLOW** [▶] to bring up the *MODFLOW* model wrapper dialog.
- 5. Once MODFLOW-USG has finished, turn on *Read solution on exit* and *Turn on contours (if not on already)*.
- 6. Click **Close** to import the solution and exit the *MODFLOW* dialog.

Notice that the contours for the computed MODFLOW heads are now visible (Figure 4), however, the targets for the observations wells are not displayed. The data for MODFLOW-USG observations must be generated and saved with the project for these calculations to occur.



Figure 4 Imported solution after initial MODFLOW-USG run

2.2 Defining Observation Data

To create the MODFLOW-USG observation input data, use the following steps:

- 1. Select *MODFLOW* | **Observations...** to bring up the *MODFLOW-USG Observations* dialog.
- 2. Select "Wells" from the list on the left.
- 3. Click **Generate PEST Obs. Data...** to bring up the *Generate Observations* dialog.

- 4. In the Head Observation Coverages section, turn on "Observation Wells".
- 5. In the Flow Observation Coverages section, turn on "Sources & Sinks".
- 6. Click **OK** to generate the observation input data and exit the *Generate Observations* dialog.
- 7. Click **OK** to exit the *MODFLOW-USG Observations* dialog.

2.3 Resaving the Project and Running MODFLOW-USG

Now that the observation data is part of the model setup, save and rerun MODFLOW.

- 1. Save 🖬 the project.
- 2. Click **Run MODFLOW** to bring up the *MODFLOW* model wrapper dialog.
- 3. Once MODFLOW-USG finishes running, turn on *Read solution on exit* and *Turn on contours (if not on already).*
- 4. Click **Close** to import the solution and close the *MODFLOW* dialog.

Notice that the calibration targets now appear (Figure 5).



Figure 5 Calibration targets are now visible

2.4 Running Pest

The original MODFLOW-2000 model included in the initial project had parameters defined. These parameters were copied to the MODFLOW-USG model. To run PEST, change the model run type to "Parameter Estimation."

- 1. Select *MODFLOW* | **Global Options...** to bring up the *MODFLOW Global/Basic Package* dialog.
- 2. In the *Run options* section, select *Parameter Estimation*.
- 3. Click **OK** to exit the *MODFLOW Global/Basic Package* dialog.
- 4. Save 🖬 the project.
- 5. Click **Run MODFLOW** [▶] to bring up the *MODFLOW/PEST Parameter Estimation* dialog.
- 6. Once PEST has finished, turn on *Read solution on exit* and *Turn on contours (if not on already).*
- 7. Click **Close** to import the solution and close the *MODFLOW/PEST Parameter Estimation* dialog.

Notice that most of the observation well targets are green, indicating that the computed value is acceptable (Figure 6). The calculated error norms can now be inspected.



Figure 6 Observation well targets are mostly green

8. Right-click on "I mfusg_pest (MODFLOW)" in the Project Explorer and select **Properties...** to bring up the *Properties* dialog.

This dialog displays the model residuals for head and flow as well as the weighted residuals for the combination of head and flow. The *Sum of Squared Weighted Residual* (Head + Flow) for this model should be approximately "11.44".

- 9. Click **OK** to exit the *Properties* dialog.
- 10. Save 🖬 the project.

3 MODFLOW–USG with PEST

3.1 Importing a Project with Pilot Points

Pilot points can also be used with MODFLOW-USG and PEST. This tutorial will import a MODFLOW-USG model with pilot points and run PEST. For more information about pilot points, refer to the "MODFLOW – PEST Pilot Points" tutorial.

- 1. Select *File* / **New** command to reset back to defaults.
- 2. Click **Open** \overrightarrow{l} to bring up the *Open* dialog.
- 3. Select "Project Files (*.gpr)" from the *Files of type* drop-down.
- 4. Select "mfusg_pilot.gpr".
- 5. Click **Open** to import the project and close the *Open* dialog.

The imported project should appear similar to Figure 7. This is a MODFLOW-USG model of the same area, but with a quadtree grid. The grid is refined around the pumping wells, river, and specified head boundary. The red points are 2D scatter points that will be used as pilot points to estimate the HK of the model.



Figure 7 Quadtree model with pilot points

3.2 Running Pest

The current model is a forward run and must be changed to the *Parameter Estimation* option to run PEST.

- 1. Select *MODFLOW* | **Global Options...** to bring up the *MODFLOW Global/Basic Package* dialog.
- 2. In the Run options section, select Parameter Estimation.
- 3. Click **OK** to exit the *MODFLOW Global/Basic Package* dialog.
- 4. Select *MODFLOW* | **Parameter Estimation...** to bring up the *PEST* dialog.

Notice that in the *Parallel PEST* section, *Use Parallel PEST* is turned on. Parallel PEST will be used to calibrate this model. Now to save the project and run PEST.

- 5. Click **OK** to exit the *PEST* dialog.
- 6. Select *File* | **Save As...** to bring up the *Save As* dialog.
- 7. Enter "mfusg_pilot_pest.gpr" as the *File name*.
- 8. Click **Save** to save the project under the new name and close the *Save As* dialog.

- 9. Click **Run MODFLOW** [▶] to bring up the *MODFLOW/PEST Parameter Estimation* dialog.
- 10. Once parallel PEST finishes, turn on *Read solution on exit* and *Turn on contours* (*if not on already*).
- 11. Click **Close** to import the solution and close the *MODFLOW/PEST Parameter Estimation* dialog.

Notice that all of the observation well targets match the model outputs, with no visible colors on the targets (Figure 8).



Figure 8 Observation well targets match the model outputs

The calculated error norms can now be inspected.

12. Right-click on "I mfusg_pilot_pest (MODFLOW)" in the Project Explorer and select **Properties...** to bring up the *Properties* dialog.

This dialog shows the model residuals for head and flow as well as the weighted residuals for the combination of head and flow. The *Sum of Squared Weighted Residual* (*Head* + *Flow*) for this model should be approximately "0.01".

- 13. Select **OK** to exit the *Properties* dialog.
- 14. Save 🖬 the project.

4 Importing a Project to Use with SVD Assist

PEST has tools for working with models that have hundreds of parameters. This PEST tool is called SVD Assist. SVD Assist can also be used with MODFLOW-USG models. The final step in this tutorial uses a model with over 200 parameters and use PEST SVD Assist to calibrate the model.

- 1. Select *File* / **New** to reset back to defaults.
- 2. Click **Open** is to bring up the *Open* dialog.
- 3. Select "Project Files (*.gpr)" from the *Files of type* drop-down.
- 4. Select "mfusg_svda.gpr" and click **Open** to import the project and exit the *Open* dialog.

The imported project should appear similar to Figure 9.



Figure 9 Voronoi grid with refinement

This is a MODFLOW-USG model of the same area, but using a Voronoi grid. The grid is refined around the pumping wells, river, and specified head boundary. The observation well locations were used to generate the grid, and each observation well is placed at the center of a cell. The blue points are 2D scatter points that will be used as pilot points to estimate the HK of the model.

4.1 Running Pest

The current model is a forward run and must be changed to the *Parameter Estimation* option to run PEST.

- 1. Select *MODFLOW* | **Global Options...** to bring up the *MODFLOW Global/Basic Package* dialog.
- 2. In the Run options section, select Parameter Estimation.
- 3. Click **OK** to exit the MODFLOW Global/Basic Package dialog.
- 4. Select *MODFLOW* | **Parameter Estimation...** to bring up the *PEST* dialog.

Notice that in the *Parallel PEST* section, *Use Parallel PEST* is turned on. Parallel PEST will be used to calibrate this model. Also notice that in the *SVD options* section, *Use SVD-Assist* is turned on.

Now to save the project and run PEST.

- 5. Click **OK** to exit the *PEST* dialog.
- 6. Select *File* | **Save As...** to bring up the *Save As* dialog.
- 7. Enter "mfusg_svda_pest.gpr" as the *File name*.
- 8. Click Save to save the project under the new name and close the Save As dialog.
- 9. Click **Run MODFLOW** [▶] to bring up the *MODFLOW/PEST Parameter Estimation* dialog.

When using SVD Assist, PEST will first run the model one time for every parameter. The information generated from that first run is used to make groups of super parameters that are then estimated by PEST. Notice that the first parameter estimation iteration required 235 model runs and that the subsequent iterations only require 11 model runs.

- 10. Once Parallel PEST finishes, turn on *Read solution on exit* and *Turn on contours* (*if not on already*).
- 11. Click **Close** to import the solution and close the *MODFLOW/PEST Parameter Estimation* dialog.

Notice that all of the observation well targets match the model outputs, with no visible colors on the targets (Figure 10). The calculated error norms can also be inspected.

12. Right-click on "I mfusg_svda_pest (MODFLOW)" in the Project Explorer and select **Properties...** to bring up the *Properties* dialog.

This dialog shows the model residuals for head and flow as well as the weighted residuals for the combination of head and flow. The *Sum of Squared Weighted Residual* (*Head* + *Flow*) for this model should be approximately "1.85".

- 13. Select **OK** to exit the *Properties* dialog.
- 14. Save 🖬 the project.



Figure 10 Observation well targets and model outputs match

5 Conclusion

This concludes the "MODFLOW-USG – PEST" tutorial. The following key topics were discussed and demonstrated:

- PEST can be used with MODFLOW-USG.
- Parallel PEST, Pilot points, and SVD Assist can also be used with MODFLOW-USG.