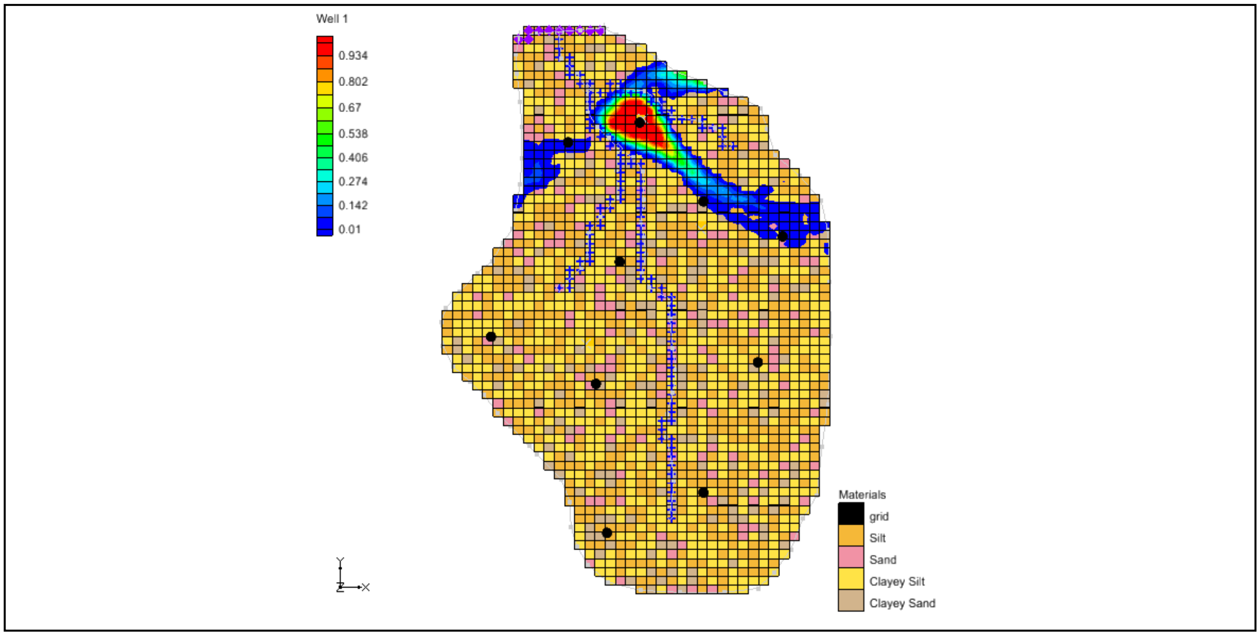
v. 9.2

GMS 9.2 Tutorial

MODFLOW – Stochastic Modeling, Inverse

Use PEST to calibrate multiple MODFLOW simulations using material sets



Objectives

The Stochastic inverse modeling option for MODFLOW is described. Multiple MODFLOW models with equally probable “realizations” of the aquifer stratigraphy are calibrated. This approach is demonstrated using the LPF and HUF packages.

Prerequisite Tutorials

- MODFLOW - Advanced PEST
- MODFLOW - Stochastic Modeling, Indicator Simulations

Required Components

- Grid
- Map
- MODFLOW
- PEST
- Parallel PEST
- Stochastic Modeling

Time

- 30-60 minutes

1 Contents

2 Introduction

GMS supports three methods for performing stochastic simulations: parameter randomization, indicator simulations and PEST Null Space Monte Carlo. These approaches are described in separate tutorials. This tutorial will use the indicator simulation approach in conjunction with PEST to create multiple calibrated MODFLOW models. With the indicator simulation approach, multiple equally probable "realizations" of the aquifer stratigraphy are generated. These realizations represent different distributions of material (indicator) zones within the aquifer. A set of aquifer properties is associated with the materials and the model is run once for each of the N realizations.

In GMS, the multiple realizations of the aquifer heterogeneity are typically generated using the T-PROGS software. T-PROGS can be used to generate two types of output: multiple material sets (arrays of material ids), or multiple MODFLOW HUF input sets. For this tutorial we will be using a pre-defined set of material sets generated by T-PROGS. The steps involved in running a T-PROGS simulation are described in the *T-PROGS* tutorial.

2.1 Outline

This is what you will do:

1. Open a MODFLOW model using the LPF package.

2. Run PEST in stochastic inverse mode.

3. Run Parallel PEST with SVD Assist in stochastic inverse mode.
4. View probabilistic capture zones.
5. Open a MODFLOW model using the HUF package.
6. Run PEST in stochastic inverse mode.

3 Description of Problem

A groundwater model for a medium-sized basin is shown in Figure 1. The basin encompasses 72.5 square kilometers. It is in a semi-arid climate, with average annual precipitation of 0.381 m/yr. Most of this precipitation is lost through evapotranspiration. The recharge which reaches the aquifer eventually drains into a small stream at the center of the basin. This stream drains to the north and eventually empties into a lake with elevation 304.8 m. Three wells in the basin also extract water from the aquifer. The perimeter of the basin is bounded by low permeability crystalline rock. There are ten observation wells in the basin. There is also a stream flow gauge at the bottom end of the stream.

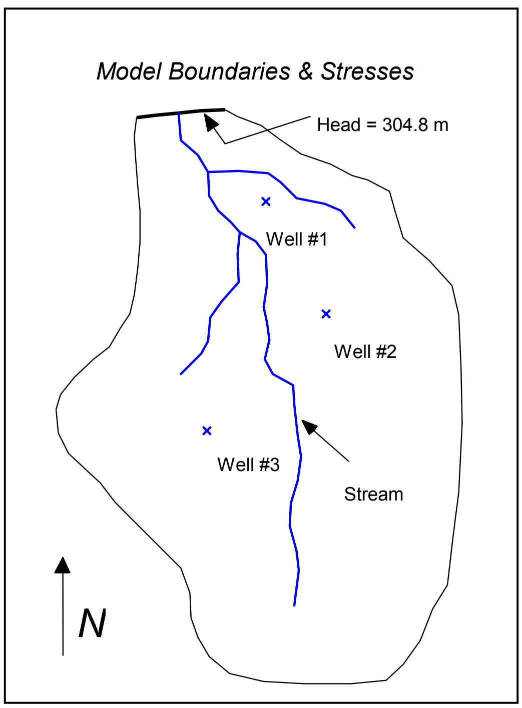


Figure 1. Sample model used in calibration exercise.

Multiple realizations of the aquifer properties have been generated.

4 Getting Started

Let's get started.

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

5 Reading in the Project

First, we will read in a project containing the MODFLOW model and the material sets generated by T-PROGS:

1. Select the *Open* button.
2. Locate and open the **Tutorials\MODFLOW\sto_inv_matset** directory.
3. Open the file entitled **lpf.gpr**.

You should see a one layer MODFLOW model showing a four-material distribution. We will now view the different material sets generated by T-PROGS:

4. Expand the following items in the *Project Explorer*: *3D Grid Data* folder, *grid (1)*, the *Material Sets* folder, and the *TPROGS* folder and the *TPROGS_A* folder.
5. Click on any of the material sets labeled **TPROGS X** (or **TPROGS_A X**). You may wish to use the up and down arrow keys on your keyboard to cycle through the material sets.

6 The MODFLOW Model Data

Most of the MODFLOW data for our model (boundary conditions, well pumping rate, top and bottom elevations, etc.) has already been entered. We will review the MODFLOW data that are somewhat more unique to this type of simulation.

1. Select the *MODFLOW* | *LPF - Layer Property Flow* command.

At the top of the dialog, notice that the *Use material ids* option is selected for the *Layer property entry method*. This means that we will not enter an array of K (hydraulic conductivity) values as is normally the case with MODFLOW. Rather, we will use material ids to define the K values.

2. Select the *Material IDs* button.

This dialog illustrates the material IDs assigned to cells. These material IDs are inherited from the active material set generated by T-PROGS.

3. Select the *OK* button to exit the *Material IDs* dialog.

4. Select the *Material Properties* button.

This dialog is used to assign aquifer properties, including hydraulic conductivity, to each of the materials used by the model. Notice that a *key* value has been assigned for Horizontal k for each material. We have also defined parameters that are being used with the materials. When the MODFLOW model is saved to disk, GMS uses the array of material IDs, the list of material properties, and the parameters to automatically generate the array of K values required by MODFLOW.

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

6. Select the *MODFLOW | Parameters* dialog.

Notice that we have 4 parameters that correspond to the four materials that are assigned to the model grid.

7. Select *OK* to exit the dialog.

7 Selecting the Stochastic Option

Before running MODFLOW, we need to turn on the appropriate stochastic simulation options. First, we will select the stochastic inverse run option:

1. Select the *MODFLOW | Global Options* command.

2. In the *Run Options* section of the dialog, select the *Stochastic Inverse Model* option.

3. Choose *OK* to exit the dialog.

Next, we need to specify that we will be using the material set method (as opposed to HUF set) in our stochastic simulation. When we choose the material set option, we must also specify which group (folder) of material sets we wish to use. In our case, we will use the *TPROGS* folder that has only 2 simulations.

4. Select the *MODFLOW | Stochastic* command.

5. Select the *Material sets* method.

6. Verify that **TPROGS** shows up in the combo box below the *Material sets* option.

7. Choose *OK* to exit the dialog.

8 Saving the Project and Running MODFLOW

We are now ready to save the project and run MODFLOW in stochastic mode.

1. Select the *File | Save As* command.
2. Save the project with the name **lpf_sto.gpr**.
3. Select the *MODFLOW | Run MODFLOW* command.

PEST and MODFLOW are now running in stochastic inverse mode. As each model run finishes, the spreadsheet on the lower right will indicate the number of PEST iterations, the model error, and the parameter values. Depending on the speed of your computer the simulation should finish in a few minutes to 20 minutes.

9 Reading in and Viewing the MODFLOW Solutions

Once all the MODFLOW runs are completed, you can read in the solutions.

1. Make sure the *Read solution on exit* toggle is checked and select the *Close* button.
2. Select *OK* at the prompt to read in all converged solutions.

You should see a new folder named **lpf_sto (MODFLOW)(STO)** appear in the *Project Explorer*. You may wish to expand this folder and view the individual solutions. You will notice that the contours vary greatly depending on the distribution of materials. As you view a particular solution, notice that the material set is updated to correspond to the material set used to generate that particular solution.

10 Running PEST SVD Assist

Instead of specifying a single value for each material, we can use pilot points to estimate the HK of each material. With early versions of PEST specifying pilot points and then undertaking a stochastic inverse model would have taken too much time because of the number of model runs required. However, SVD-Assist greatly reduces the number of required runs and we can further speed up the process by using Parallel PEST.

First, we will assign pilot points to the parameters. Then we will turn on Parallel PEST and SVD Assist.

1. Select the *MODFLOW | Parameters* command.
2. Select the drop down arrow in the *Value* column for the **HK_Sand** parameter and select <*Pilot points*>.
3. Select the button above the drop down arrow in the *Value* column for the **HK_Sand** parameter. This will bring up the pilot point options dialog.

4. In the *Data section* at the top of the dialog, make sure that the *Data set* is set to **sand** and then select OK to exit the dialog.

5. Repeat this process for the other parameters and make sure to select the appropriate data set in the pilot point options dialog.

6. Select *OK* to exit the Parameters dialog.

7. Select the *MODFLOW | Parameter Estimation* command.

8. Turn on *Use Parallel PEST*, *Use SVD*, and *Use SVD-Assist*.

9. Select *OK* to exit the dialog.

11 Saving the Project and Running MODFLOW

We are now ready to save the project and run MODFLOW in stochastic mode.

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

2. Save the project with the name **lpf_sto1.gpr**.

3. Select the *MODFLOW | Run MODFLOW* command.

Parallel PEST and MODFLOW are now running in stochastic inverse mode. On a reasonably fast multi-core processor, this run should finish in about 5 minutes.

12 Reading in and Viewing the MODFLOW Solutions

Once all the MODFLOW runs are completed, you can read in the solutions.

1. Make sure the *Read solution on exit* toggle is checked and select the *Close* button.

2. Select *OK* at the prompt to read in all converged solutions.

You should see a new folder named **lpf_sto1 (MODFLOW)(STO)** appear in the *Project Explorer*. You may wish to expand this folder and view the individual solutions. Notice that the observation targets for these new results match much better than the previous stochastic inverse run.

13 Probabilistic Capture Zones

We will now read in the results from a stochastic inverse run using the **TPROGS_A** material sets.

1. Select the *MODFLOW | Read Solution* command.

2. Locate and open the **Tutorials\MODFLOW\stochastic3\run1_MODFLOW** directory.

3. Select **run1.mfn** and select *OK*.

4. Select OK to read in all of the solutions.

You should see a new folder named **run1 (MODFLOW)(STO)** appear in the *Project Explorer*.

5. Right click on the **run1 (MODFLOW)(STO)** in *Project Explorer* and select the *Risk Analysis* command.

6. Select the *Probablistic capture zone analysis* option and select the *Next* button.

7. Select the *Finish* button to run the analysis.

MOPATH is now running in the background. You should see a progress bar update as MODPATH is run for each of the simulations in the stochastic solution. When MODPATH is finished running, GMS will create a new data set for each well in the model. We can view the probability of capture from each cell to each well in the model.

8. Expand the **Display Themes** in the *Project Explorer* and select the **color fill contours** display theme.

You should now see contours (similar to the next figure) showing the probabilistic capture zone for the well near the top of the model.

Figure 2 Probabilistic Capture Zone for a well

14 Stochastic Inverse with HUF

The stochastic inverse approach can also be used with multiple HUF data sets. We will now read in a project with multiple HUF data sets and run a stochastic inverse model.

1. Select the *File* | *New* command to reinitialize the project.
2. Select the *File* | *Open* command.
3. Locate and open the **Tutorials\MODFLOW\sto_inv_matset** directory.
4. Open the file entitled **huf.gpr**.

You should see the same model that we have been working with. However, this model uses the HUF package instead of the LPF package. If you select a grid cell and then change to side or front view you will see the different hydrogeologic units defined in the HUF package similar to what is shown in the figure below.

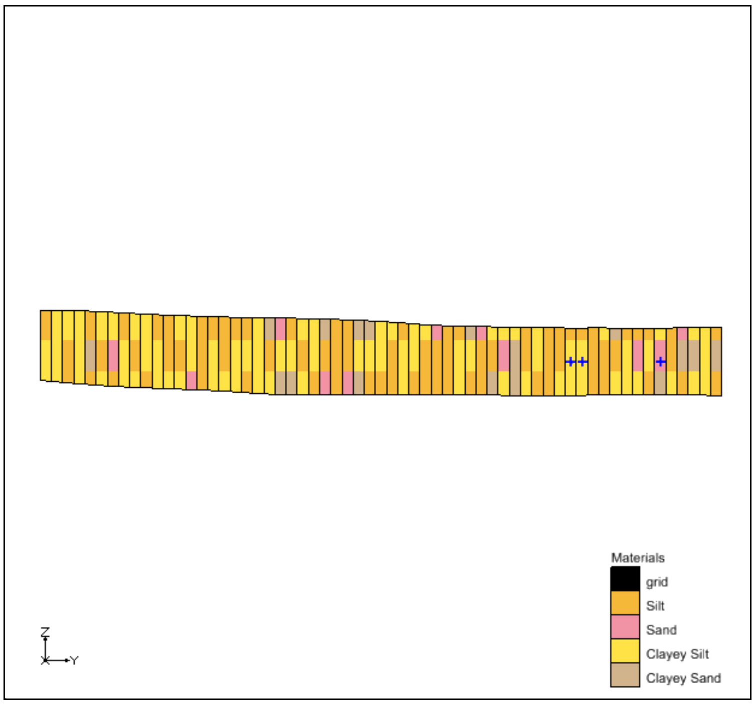


Figure 3 Hydrogeologic units from the HUF package

5. Select the *MODFLOW* | *Global Options* command.
6. In the *Run Options* section of the dialog, select the *Stochastic Inverse Model* option.
7. Choose *OK* to exit the dialog.
8. Select the *MODFLOW* | *Stochastic* command.

9. Select the *HUF sets* method.
10. Verify that **TPROGS** shows up in the combo box below the *HUF sets* option.
11. Choose *OK* to exit the dialog.
12. Select the *File* | *Save As* command.
13. Save the project with the name **huf_sto.gpr**.
14. Select the *MODFLOW* | *Run MODFLOW* command.

Parallel PEST and MODFLOW are now running in stochastic inverse mode. On a reasonably fast, multi-core processor, this run should finish in about 5 minutes.

15 Reading in and Viewing the MODFLOW Solutions

Once all the MODFLOW runs are completed, you can read in the solutions.

1. Make sure the *Read solution on exit* toggle is checked and select the *Close* button.
2. Select *OK* at the prompt to read in all converged solutions.

You should see a new folder named **huf_sto (MODFLOW)(STO)** appear in the *Project Explorer*. You may wish to expand this folder and view the individual solutions. As you view a particular solution, notice that the HUF data is updated to correspond to the HUF set used to generate that particular solution.

16 Conclusion

This concludes the Stochastic Modeling – Inverse tutorial. Here are the things that you should have learned in this tutorial:

- You can calibrate multiple models using the Stochastic inverse modeling option.
- The stochastic inverse modeling approach supports material sets and HUF set.
- Material sets and HUF sets can be created using TPROGS.
- The *Risk Analysis Wizard* can be used to do a probabilistic capture zone analysis.