

GMS 10.0 Tutorial MODFLOW – Stochastic Modeling, PEST Null Space Monte Carlo II

Use results from PEST NSMC to evaluate the probability of a prediction



Objectives

Learn how to use the results from a PEST Null Space Monte Carlo (NSMC) simulation to set up a new stochastic simulation with MODFLOW.

Prerequisite Tutorials

 MODFLOW – Stochastic Modeling, PEST Null Space Monte Carlo I

Required Components

- Grid Module
- Map Module
- MODFLOW
- PEST
- Stochastic Modeling
- Time

• 35-50 minutes

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1 Introduction

GMS supports the following three methods for performing stochastic simulations:

- Parameter randomization
- Indicator simulations (T-PROGS)
- PEST Null Space Monte Carlo (NSMC)

The first two approaches are described in separate tutorials. This tutorial will explain features of GMS associated with the PEST NSMC method. If the user has not done so already, it is highly recommended that the user finish the "MODFLOW – Stochastic Modeling, PEST Null Space Monte Carlo I" tutorial prior to doing this tutorial.

The "MODFLOW – Stochastic Modeling, PEST Null Space Monte Carlo I" tutorial discussed how the NSMC method is used to create multiple calibrated MODFLOW models. This exercise is useful for exploring the uncertainty associated with the calibrated model. However, a groundwater model is normally used to help make some kind of future prediction. The usual process for using a model to make a prediction is as follows: first, use historical data to create a calibrated groundwater model; second, modify the calibrated model to account for some future scenario and evaluate the prediction.

For example, perhaps the user wants to know how much drawdown a well would cause if an area was in a drought for a prolonged period of time. First, the user would create a calibrated groundwater model using historical information on water levels, pumping rates at wells, and rainfall. Then, the user would take the calibrated model as a starting point, modify the inputs so as to simulate a drought, and then run the model. The user could then view the model outputs and make a prediction on the amount of drawdown caused by a well in such a scenario.

It could never be said that the user would be 100% confident in this prediction because uncertainty is associated with various inputs to the groundwater model—hydraulic conductivity, recharge, water levels, etc. All have error associated with their input values. More often than not, the model is better than a scientific guess since, in building the model, the user has analyzed the study area and accounted for the different processes that affect groundwater. Further, the user has used historical data to make sure that the model can match what has been measured in the past. So while the model is not perfect, it is better than a less sophisticated approach.

Using the NSMC method, the user now has a method for quantifying the amount of uncertainty associated with the prediction. Instead of creating a single calibrated model, the user can use PEST NSMC to create multiple calibrated models. The user can modify the model to account for future conditions and then run multiple models using the different parameter values that PEST calculated. Then the user can view a distribution of results for this prediction. Using the previously mentioned drawdown example, the user can present a mean drawdown with a standard deviation instead of presenting a single value. In this way, the user can feel much more confident in the prediction. If the amount of uncertainty associated with the prediction. If the amount of uncertainty is unacceptably high, then more work may be required, such as collecting more field data or better calibrating the original model.

1.1 Outline

Here are the steps of this tutorial:

- 1. Open a project with multiple calibrated MODFLOW solutions that were calibrated using PEST NSMC.
- 2. Modify the MODFLOW simulation.
- 3. Set up a stochastic run using the results from PEST NSMC.
- 4. Run MODFLOW in stochastic mode.

2 Description of Problem

A groundwater model for an unconfined alluvial aquifer in Wisconsin, USA, is shown in Figure 1. The alluvium is highly variable in terms of hydraulic conductivity. In some areas, it is composed of high conductivity, well-sorted gravels, while in other areas, it is composed of low conductivity, sandy silts. While the location and description of the model area are accurate, the observation wells used in this exercise are not field-measured values.



Figure 1 Study area

The model is bounded on the east by Lake Wisconsin and on the south by the Wisconsin River. A stream (Otter Creek) is used as the western boundary. Based on observed heads, it is assumed that there is a significant amount of recharge occurring along the northern boundary. The aquifer becomes very thin as on the northern and western boundaries.

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 a project containing the MODFLOW solution:

- 1. Select the **Open** 😂 button.
- 2. Locate and open the *Tutorials\MODFLOW\sto_pest_nsmc_II* directory.

- 3. Select the file entitled "nsmcII.gpr."
- 4. Click **Open.**

The user should see a one-layer MODFLOW model and observation wells similar to the figure below.



Figure 2 Calibrated MODFLOW model

- 5. Expand the following items in the Project Explorer:
 - "3D Grid Data" 🗇 folder
 - "grid" 🕮 item
 - "nsmcII (MODFLOW)(STO)" 📮 folder.

These are the results from a PEST Null Space Monte Carlo run. The current set of heads are part of the nsmcII001 (MODFLOW) solution. The user may wish to select different solutions to see the variability in the computed heads.

6. Double-click on the "nsmcII.mfo" 🗒 text item in the Project Explorer.

This will open this file in a text editor. The user should see something similar to the figure below.

Figure 3 Stochastic output file (nsmcll.mfo) displayed in Notepad

This file describes the PEST NSMC run. If the user scrolls through the file, he or she will see that this stochastic simulation comprised 30 different models. Each line in the file describes a model run. Notice that the name of the simulation, the number of PEST iterations, the model error, and the parameter values are given on each line.

The original calibrated model had a total model error of 197.5. During the NSMC run, PEST would run each model until the total model error was less than 200.0 (the value specified for the PEST input parameter PSTOPTHRESH). Model runs 2, 10, and 21 had model error above the 200.0 and so they were removed from the stochastic folder in the project explorer. Model run 29 encountered some kind of problem so it was reported as a failed run.

7. Close the text file and return to GMS.

5 The MODFLOW Run Options

Now the user will modify the MODFLOW run to analyze the capture zone of a proposed well. Then the user will run MODFLOW in stochastic mode using the results from the PEST NSMC run.

1. Select the *MODFLOW* | **Global Options** command to open the *MODFLOW Global/Basic Package* dialog.

- 2. Under the Run options section of the dialog, select the Stochastic option.
- 3. Select the **Stochastic Options** button to open the *Stochastic Options* dialog.

This dialog is used to change the stochastic options. The user is still going to use the PEST NSMC option, but it is necessary to select the PEST NSMC stochastic solution that will be used as input for the new stochastic simulation.

- 4. In the drop down box next to the *PEST NSMC* option, select the "nscmII (MODFLOW)(STO)" option.
- 5. Select **OK** to exit the *Stochastic Options* dialog.
- 6. Select **OK** to exit the *MODFLOW Global/Basic Package* dialog.

6 Creating the new well

The user is now ready to add the proposed well and run MODFLOW.

- 1. Select the **Zoom** $\stackrel{\frown}{\overset{\frown}{\overset{\frown}}}$ tool.
- 2. Zoom in on the area shown in the figure below by dragging a box with the Zoom tool.



Figure 4 Area in model where new well will be created

- 3. Select the Select 3D Grid Cells 🔂 tool.
- 4. Select the cell shown in the next figure. The cell ID at the bottom of the GMS window should be 2356.



Figure 5. Location of new well.

- 5. Right-click on the cell.
- 6. Select the **Sources/Sinks** command to open the *MODFLOW Sources/Sinks* dialog.
- 7. Select *Wells* from the list box on the left side of the dialog.
- 8. Click on the Add BC button at the bottom of the dialog to create a new well.
- 9. Enter "Well 4A" for the name.
- 10. Enter "-65000.0" for the flow rate. (See the next figure)

MODFLOW Sources/Sinks						×
Wells Wells (MNW 1) Wells (MNW2) Specified Head Drain Drain (DRT) River General Head Recharge	ID All 2356	Name Well 4A	Q (flow) (ft^3/d) -65000.0			
 Display cell id Display cell I, J, K 						
Help	Add	BC	Delete BC Del	lete All BCs	ОК	Cancel

Figure 6 Sources/Sinks dialog creating a new well

- 11. Select **OK** to exit the dialog.
- 12. Select the **Frame** 🔯 macro.

7 Removing the observations

It is necessary to remove the head observations since the user is now running a model scenario that is inconsistent with these head measurements.

- 1. Select the *MODFLOW* / **Observations** command to open the *Observations* dialog.
- 2. Uncheck the *Use* toggle next to the "wells" coverage on the right side of the dialog.

Observations					8	×
Group weights		Covera	ges (head ob	servations)		
Head observations:	1.0	Use	Coverage	Measurement		
Constant head flow observations:	1.0		wells	Head	_	_
River flow observations:	1.0					
General head flow observations:	1.0					
Drain flow observations:	1.0					
Drain (DRT) flow observations:	1.0					
Stream flow observations:	1.0					
Dry value for cells (HOBDRY):	-777				Export	Trans. Obs
Note: Head and flow observations a	re defined using observatio	on and sou	rce/sink cov	erages in the Map r	nodule.	
Help					ОК	Cancel

Figure 7 Observations dialog

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

8 Saving the Project and Running MODFLOW

Now save the project and run PEST in stochastic mode.

- 1. Select the *File* | **Save As** command.
- 2. Change the project name to "nsmcII_forward.gpr."
- 3. Click Save.
- 4. Select the *MODFLOW* | **Run MODFLOW** command.

MODFLOW is now running in stochastic mode as shown in the next figure. Depending on the speed of the user's computer this process may take up to 15 minutes. On a fairly fast computer, the model should finish running in a couple of minutes.

🕝 Stoo	hastic MODFL	ow					×			
Finished										
	Converged	rah 601	mb 602	div 501	aa1v1	aa1w10	aa1v11 .			
Run	1 YES	0.001	0.00079999998	0.061269	12.71415	5.803843	2.88558			
Run	2 YES	0.001	0.00079999998	0.061269	0.5	22.10578	0.5			
Run	3 YES	0.001	0.00079999998	0.061269	12.6291	285.0204	0.604629			
Run	4 YES	0.001	0.00079999998	0.061269	400.0	400.0	0.5			
Run	5 YES	0.001	0.00079999998	0.061269	400.0	400.0	0.5 👻			
Total	lanced time : 0 br	re () min 56								
Totare	apsed time. o ni	5 0 min 50	360							
Run	start date an	nemell f	vvvv/mm/dd hh:m	m:ss): 20	12/07/26 1	0:14:39				
Finis	Finished iteration 1 of timestep 1 of period 1									
Finis	shed iteration	1 3 0	f timestep	1 of perio	od 1					
Finis	shed iteration	n 4 o:	f timestep	1 of perio	od 1					
Finis	shed iteration	1 5 o: 6 o:	f timestep f timester	1 of perio	od 1					
Finis	shed iteration	1 7 0	f timestep	1 of perio	od 1					
Finis	shed iteration	n 8 o:	f timestep	1 of perio	od 1					
т	TAL SUM OF S	QUARED, WI	EIGHTED RESIDUA	LS: 0.6511	6-24					
Run end date and time (yyyy/mm/dd hh:mm:ss): 2012/07/26 10:14:39 Elapsed run time: 0.325 Seconds										
MODFLOW 2000 terminated successfully										
Stochastic runs finished.										
Help I Read solution on exit I Turn on contours (if not on already)										

Figure 8 PEST Model Wrapper

The spreadsheet (outlined in red above) shows the parameter values for each model run and whether or not the model converged. Below the graph is a text window (outlined in blue above) that shows the output that MODFLOW would print to the screen if the user were running MODFLOW from the command line.

For each model run, GMS reads the parameter values calculated by PEST in the previous NSMC run and saves those parameter values to the SEN package file for MODFLOW 2000 or to the PVAL package file for MODFLOW 2005 and NWT. Then MODFLOW executes that model run.

9 Reading in and Viewing the MODFLOW Solutions

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

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

The user should see a new folder named "nsmcII_forward (MODFLOW)(STO)" in the Project Explorer. Expand this folder and view the individual solutions.

10 Risk Analysis

Now use the nsmcII_forward set of stochastic solutions to examine the capture zone for the new well.

- 1. Right-click on the "nsmcII_forward (MODFLOW)(STO)" folder in the Project Explorer.
- 2. Select the **Risk Analysis** command.
- 3. Select the *Probabilistic capture zone analysis* option.
- 4. Then click the **Next** button.
- 5. Under the *Particle termination at cells with weak sinks* section, select the *Stop in cells with weak sinks* option.
- 6. Select the **Finish** button.

GMS is now running MODPATH on each of the MODFLOW solutions. A particle is placed on the water table surface at each cell in the model grid and then the particle is tracked forward in time to determine the cell where the particle terminates. When the model finishes running, the user should see something similar to the figure below.



Figure 9 Probabilistic capture zone for proposed well

The figures below show capture zones from individual solutions computed by MODFLOW. Notice the difference in the shape and location of the various capture zones. This is due to the uncertainty associated with this model. Even though the model has been calibrated to field measured water level data, using PEST NSMC the user can create multiple calibrated models that show significant differences in the capture zone for the well. Thus, it is more reasonable to discuss modeling results in terms of uncertainty and probability than in terms of the results from a single model.



Figure 10 Capture zones from individual runs

11 Conclusion

This concludes the *Stochastic Modeling – PEST Null Space Monte Carlo II* tutorial. Here are the key concepts in this tutorial:

- It is possible create a new stochastic solution using the results of a completed PEST Null Space Monte Carlo run.
- The Risk Analysis tools in GMS allow the user to create probabilistic capture zones.