**Extension of AnAqSim in Depth, Session 6 Exercise**

Dave Dahlstrom
Barr Engineering Co.

This document explains how modeling tasks such as the pumping optimization exercise in Step 21 of the Session 6 Exercises can be automated. The software PEST was used. PEST is free and is found at this URL:

http://www.pesthomepage.org/Downloads.php

Copies of the PEST executable and the small subset of its utility programs used in this application are included in the .zip file. Refer to the manuals distributed with PEST for more information (included in the zip file as *newpestman1.pdf* and *newpestman2.pdf*).

Note that there is also a commercial version of PEST called PEST_HP that provides even more robust optimization algorithms than the free version. For more information, see:

https://pest.cloud/

# Introduction to PEST

PEST is an extremely powerful suite of software for model calibration and prediction uncertainty quantification. PEST is model-independent; it can be applied to any model which has the following attributes:

- text-based input files to which PEST can write its parameter values to using template files,
- text-based output files that PEST can read its observations from using instruction files, and
- the ability to run the model using a DOS batch file.

AnAqSim has all of these attributes. Details of the application are described below.

# Add Transient Head Observations in AnAqSim

The following changes were made to the file created during the exercise, which is named *transient2_adj_2sp.anaq*.

In AnAqSim, digitize the location of the X shown on p.5/7 of the Exercise 6 pdf (the point near the flow barrier where the highest heads are simulated).

Then select Analysis Input | Calibration Targets | Head

Add four observations at this x,y location – the head at the end of each time period in the simulation in levels 1 and 2. The goal of the optimization is to have all of these heads below 27.0 head units by t=5 time units and to keep the heads below 27.0 through the end of the simulation at t=21.

Also add four observations at the center of the area within the barrier (copy the coordinates from one of the hydrograph points at that location). The screen capture below shows the calibration heads in the model:

Data: calibration heads

| Label | Level | X,Y | Observed_Head | Time | Show |
|---|---|---|---|---|---|
| in_barrier_L1_t5 | 1 | -13.2439118548158, 16.1906527187793 | 27.0 | 5.0 | ☑ |
| in_barrier_L1_t21 | 1 | -13.2439118548158, 16.1906527187793 | 27.0 | 21.0 | ☑ |
| in_barrier_L2_t5 | 2 | -13.2439118548158, 16.1906527187793 | 27.0 | 5.0 | ☑ |
| in_barrier_L2_t21 | 2 | -13.2439118548158, 16.1906527187793 | 27.0 | 21.0 | ☑ |
| center_L1_t5 | 1 | 13.4367833224132, -41.0054320012279 | 27.0 | 5.0 | ☑ |
| center_L1_t21 | 1 | 13.4367833224132, -41.0054320012279 | 27.0 | 21.0 | ☑ |
| center_L2_t5 | 2 | 13.4367833224132, -41.0054320012279 | 27.0 | 5.0 | ☑ |
| center_L2_t21 | 2 | 13.4367833224132, -41.0054320012279 | 27.0 | 21.0 | ☑ |

## Automate Execution of AnAqSim

Execution of AnAqSim runs from the command line is described in Section 4 of the User Guide. In this case, AnAqSim is run from the command line using the following command:

"c:\program files\fitts geosolutions\anaqsim\anaqsim.exe" transient2_adj_2sp.anaq run_anaqsim.txt

Modification of the file *transient2_adj_2sp.anaq* by the PEST utility OBS2OBS to optimize the pumping is described below. The AnAqSim run control file *run_anaqsim.txt* indicates which starting heads file to use for the transient simulation (created during the exercise), the name of the output file where the observations of interest are written, and other aspects of the execution. The calibration heads are the only aspect of the run used by PEST in this case.

The AnAqSim outputs are written to the file *transient2_adj_2sp.out*.

## Applying PEST to the Optimization Problem

The problem is to find the optimal system discharges that will keep heads at or below 27 at all points within the barrier in levels 1 and 2 from t=5 to the end of the simulation at t=21.

Remember that the combined pumping rate of the multi-domain pumping wells is injected in the recharge trench. So this problem has two parameters that will be optimized:

1. The pumping rate per multi-domain well in time period 1
2. The pumping rate per multi-domain well in time period 2

Calculation of the injection rate as the well pumping rates change during the optimization is described below.

### PEST template files

AnAqSim input files (.anaq extension) are written in .xml format, so are readily replicated/modified using PEST template files. The file *transient2_adj_2sp.anaq* is created using the template named *transient2_adj_2sp.anaq.tpl*. The header line "ptf" identifies the file as a PEST template file and the $

character is used to delineate where PEST or PEST utilities will write parameter values. Execute this command to get a listing of the parameters:

tempchek transient2_adj_2sp.anaq.tpl

The parameters are named as follows ("ext" for extraction, "inj" for injection):

ext_rate1
ext_rate2
inj_rate1
inj_rate2

The injection rates per time period are calculated based on the well pumping rates as they change during optimization run using the PEST utility PAR2PAR. See the template file *par2par_input.txt.tpl* used by PEST to write the pumping rates (ext_rate1 and ext_rate2) into the file *par2par_input.txt*. When executed, PAR2PAR reads the file *par2par_input.txt*, calculates the injections rates for time periods 1 and 2, and uses the template file *transient2_adj_2sp.anaq.tpl* to write the AnAqSim input file *transient2_adj_2sp.anaq*.

Note that PEST allows one parameter value to be tied to another value such that the ratio between the parameters remains the same, but I chose to use PAR2PAR to demonstrate how that utility program can be used.

## PEST instruction file and censored observations

Pumping during the first time period draws the heads down rapidly, then the rate can be reduced and some recovery will occur during the second time period. There will be some overshooting, i.e., drawing of heads at the end of time period 1 below the target of 27. We don't know how low they will go – we just know that they should still be below 27 at the end of time period 2. Observations of the kind at the end of time period 1 are referred to a "censored". We don't know exactly what they should be, just what they should not be (not > 27). This type of observation can be handled with a utility provided with PEST called OBS2OBS. For example, line 6 of file *obs2obs_excess_heads_tp1.rsp* returns the larger of the two values: 0.0 and (hd_x_1_5 - 27.0). If the simulated head hd_x_1_5 is less than or equal to 27, the PEST observation ex_x_1_5 will be zero, meaning the pumping objective is being met.

OBS2OBS will create an instruction file for use in reading its own output file if executed as follows (all in one line at the command prompt):

obs2obs.exe obs2obs_excess_heads_tp1.rsp obs2obs_excess_heads_tp1.out obs2obs_excess_heads_tp1.out.ins

An instruction file can be checked to make sure it is reading the observations properly using the following command:

inschek.exe obs2obs_excess_heads_tp1.out.ins obs2obs_excess_heads_tp1.out

It was noted through running the problem manually that the calibration head observation named hd_x_2_21 had the highest of any of the heads checked at the end of the simulation. Therefore, this was the only observation from the end of time period 2 to which a non-zero weight was applied – the others "come along for the ride" but do not influence the optimization (see the third entry in lines 28-31 of the file *ex6_optimiz_3.pst*).

OBS2OBS does not have if-then or similar constructs, so if you wanted to check each model run to make sure you were comparing the highest of all simulated heads at the end of time period 2 to the target head, you would have to write a program to accomplish this task. We use python scripts for these sorts of modeling tasks. When many parameters are being adjusted, PEST is usually run in parallel so be aware that portability to an array of workstations or virtual machines can be more of an issue with interpreted languages like python than with compiled programs.

PEST observation names are currently limited to 20 characters. There is no reason that the labels used in AnAqSim and the character names used by PEST could not be the same, but they are different in this application. Although the "-" character is allowed in a PEST observation name, its use in these names is not encouraged as it can interfere with usage of the utility OBS2OBS (it gets parsed as the subtraction operator).

## PEST batch file

The file *ex6_optimiz_3.bat* has all of the commands needed to accomplish the following tasks (note that by the time PEST runs this batch file, it has already created the model input file *par2par_input.txt*):

- delete intermediate files that PEST does not work with directly (good practice to facilitate troubleshooting of model setup)
- calculate injection rates for time periods 1 and 2 (done by PAR2PAR),
- write the AnAqSim input file (done by PAR2PAR),
- run AnAqSim, and
- post-process the censored observations (done by OBS2OBS).

Once the batch file returns control to PEST, PEST reads the observations it is looking for from the file *obs2obs_excess_heads_tp1.out*.

## PEST control file and run results

All of the parts described above are brought together in the file *ex6_optimiz_3.pst*. PEST is executed by typing the following at the command line:

pest ex6_optimiz_3.pst

The run record file *ex6_optimiz_3.rec* indicates the progress through the optimization. The starting pumping rates were -300 $L^3$/T per well in each time period and the target head of 27 was exceeded at all locations checked at the ends of both time periods. The optimized rate per well in time periods 1 and 2 are -987 and -601 $L^3$/T, respectively. These compare favorably with the manually-derived values of -1050 and -600 from the key to the exercise.

As required, the censored heads at the end of time period 1 are all less than 27.0 (ranging from about 26.39 to 26.87). These values are in file *transient2_adj_2sp.out*. The maximum head at the points checked in levels 1 and 2 (hd_x_2_21) equals exactly 26.999 as specified in the PEST control file. The other heads at the end of time period 2 do not equal the values specified in PEST, but, as noted above, their weights were set to zero so the optimization would be based on observation hd_x_2_21. As expected, these other heads are less that target value (see the file *ex6_optimiz_3.res*).

If you have any questions about this PEST application, you can reach me at ddahlstrom@barr.com