### MU-ATC-5: Capture Zone in a Heterogeneous Aquifer

**Test Case Description**

Test Case 5 tests mod-PATH3DU’s ability to recreate within acceptable tolerance levels a ten-year capture zone in a heterogeneous aquifer. The test it’s recreating is the same test from Test Case 4. Refer to [Section x] for information about the test to be reproduced.

**Test Case Setup**

Test setup consists of three parts:

* Assemble the MODFLOW model to serve as the underlying flow model. Use the inputs stated in ISWS/BUL-69/87 and estimate inputs when necessary.
* Assemble the MODPATH model for particle tracking. Use the inputs stated in ISWS/BUL-69/87 and estimate inputs when necessary.
* Assess the pass/fail status of the test by comparing the MODPATH results to the digitized results of Figure 3‑9.

*Assemble the MODFLOW Model*

Test Case 5 uses the MODFLOW files from Test Case 4. These files were copied from Test Case 4 during development and are not replaced with each model run, as the outputs are assumed to be the same. The only change to the MODFLOW files from Test Case 4 are the filenames (changed from “test\_case\_4” to “test\_case\_5”) and some changes to the Name file to make the data executable with mod-PATH3DU files. Though mod-PATH3DU can work with unstructured grids of any shape, it is only tested in this document on a rectilinear grid.

*Assemble the mod-PATH3DU Model*

The mod-PATH3DU model uses different files than MODPATH

1. Make the starting particle location files into a shape

*Pass/Fail Criteria*

The acceptance criteria for this test are as follows:

* Criterion 1 – The area of the capture zone created by MODPATH is within 10% difference of the capture zone in ISWS/BUL-69/87.
* Criterion 2 – The left and right extents in the x-direction, and the top and bottom extents in the y-direction, are within 10% difference of those extents in ISWS/BUL-69/87.

All percent differences are calculated from the ISWS/BUL-69/87 values.

Criterion 1 gives evidence that the overall size of the capture zone is within an acceptable range of ISWS/BUL-69/87. Criterion 2 gives evidence that the shape of the capture zone is within an acceptable range of ISWS/BUL-69/87. The pass/fail status of the criteria will be printed to a file, listed in [Section x].

**Sources of Error**

There are several sources of error in this test case.

* ISWS/BUL-69/87 was not explicit on how the flow field was created.
* The constant head values on the left and right were not explicitly stated. This, combined with the first bullet, resulted in a slightly different flow field for this test case than that seen in ISWS/BUL-69/87.
* The particle tracking was done using a node-based method, as opposed to MODFLOW and MODPATH’s cell-based method. This offset, while corrected for in the test case, still resulted in differences in the internal boundaries of the hydraulic conductivity field. This difference in the hydraulic conductivity field may adjust the shape of the flow field and the capture zone.
* The particle tracking in ISWS/BUL-69/87 was calculated using GWPATH, not mod-PATH3DU. This may have resulted in some differences in the capture zone shape.

**File Structure**

All files for Test Case 5 are contained within the “Test\_Case\_5” folder in the root directory. The structure within that folder is as follows:

* /gwpath\_digitized (This folder contains shapefiles with data digitized from figures in ISWS/BUL-69/87)
  + fig\_21\_10\_yr\_capture\_zone.shp and related files
    - Description: This is a shapefile of the capture zone, digitized from the raster version of [Figure 3-9]. Information about the raster version of [Figure 3-9] is presented later in this section. This shapefile is used in the pass/fail criteria calculation.
* /output (This folder contains the post-processing files used to determine the pass/fail status of the test case, as well as other output files)
  + /shapefiles (This folder contains shapefiles created as outputs. All the shapefiles in this folder were created by the executable “writeP3DOutput.exe”, using “out.json” and “output\_PATHLINE.bin”.)
    - Endpoint\_mp3du.shp and associated files
      * Description: This shapefile is a point file containing a point for each particle that defines where that particle is at the ten-year mark.
    - mp3du\_10\_yrs\_poly.shp and associated files
      * Description: This shapefile is a polygon of the ten-year capture zone, created by connecting the space between the points in “Endpoint\_mp3du.shp”.
    - Pathline\_mp3du.shp and associated files
      * Description: This shapefile is a line file of the particle tracks of the ten-year capture zone created in this test case.
  + mp3du.gsf
    - Description: This is the grid specification file. This file provides x- and y-coordinates for the vertices of each cell in the MODFLOW grid. This file is specific to mod-PATH3DU. This file was created by the executable writep3dgsf.exe, using the file “gsf.json”.
  + mp3du\_pathline.png
    - Description: This image file shows the particle pathlines in mod-PATH3DU that define the capture zone for this test case.
  + output\_PATHLINE.bin
    - Description: This binary file contains the particle locations. It is produced by executing the model run.
  + tc5\_results.csv
    - Description: This file contains the pass/fail results for this test case. The pass/fail results are listed in row 5, and rows 1-4 contain the information used to determine the pass/fail result.
* CHD.chk
  + Description: []
* gsf.json
  + Description: a mod-PATH3DU file that serves as an input to writep3dgsf.exe. It is used to make an output file (“mp3du.gsf”).
* MP3DU.log
  + Description: This is a log file created when mp3du.exe is executed.
* mp3du\_modflow.lst
  + Description: This is a list file created when mp3du.exe is executed.
* mp3du\_test\_case\_5.p3d
  + Description: This is the per-cell property file. It lists values for properties required by the particle tracking that may vary in each model cell, such as porosity, dispersivity, and retardation parameters.
* out.json
  + Description: This file is used by writep3doutput.exe to direct that executable to the output binary file and to define what shapefiles will be created using the data from the output binary file.
* primary.json
  + [Description: This file provides information to mp3du.exe for the mod-PATH3DU model execution. This file defines the location of the grid specification file, the MODFLOW Name file, the point starting location file, and the output folder. This file also provides other information for the model, e.g. the particle track direction.
* runme.bat
  + Description: This batch file creates the output folder and the shapefiles subfolder within it, it runs the mod-PATH3DU utilities as well as mod-PATH3DU, and it runs the post-processing python scripts.
* S01\_create\_bounding\_shp.py
  + Description: This python script assigns projection data to the shapefiles created by the executable “writeP3DOutput.exe”. This script also creates “mp3du\_10\_years\_poly.shp” from “Endpoint\_mp3du.shp”
* S02\_compare\_capturezones.py
  + Description: This script uses the area and point location data of “fig\_21\_10\_yr\_capture\_zone.shp” and “mp3du\_10\_yrs\_poly.shp” to calculate the statuses of the pass/fail criteria.
* starting\_circle.shp and related files
  + Description: This is a point shapefile with 100 equally-spaced points in a circle, at a radial distance of 15.2 m (50 ft) from the extraction well being examined (Well 3).
* test\_case\_5 and related files (file types listed in alphabetical order: BAS, CHD, DIS, LPF, NAM, OC, PCG, WEL, CBC, GLO, LIST, HDS, MPBAS, MPNAM, MPSIM, MPEND, MPLST, MPPTH)
  + Description: MODFLOW files copied from Test Case 4 and renamed. The Name file has been updated for compatibility with mod-PATH3DU.
* texas\_gam.prj
  + Description: projection data for the projection arbitrarily selected for use in this test case.
* writeP3DGSF.log
  + Description: This is a log file created when writep3dgsf.exe is executed.
* writeP3DOUTPUT.log
  + Description: This is a log file created when writep3doutput.exe is executed.
* writep3dgsf.exe
  + Description: This executable reads the file “gsf.json” and outputs “mp3du.gsf”. This executable was created by SSP&A. The file “mp3du.gsf” is exclusively used by mod-PATH3DU.