# OVERVIEW AND SCOPE

| Acronym: | MODFLOW | HISI ID: | 2517 | Software Grade: | C |
| --- | --- | --- | --- | --- | --- |
| Acronym: | MT3DMS | HISI ID: | 2518 |
| Acronym: | MODPATH | HISI ID: |  |
| Acronym: | modPATH-3DU | HISI ID: |  |

This Software Test Plan (STP) is required by PRC-PRO-IRM-309, *Controlled Software Management*, to define the testing requirements for MODFLOW (MODular finite-difference FLOW model) and related codes for CH2M HILL Plateau Remediation Company (CHPRC) intended use in risk and model integration work.

MODFLOW and related codes are managed as acquired, commercial off-the-shelf (COTS) software applications. The CHPRC plans to use this for calculations of short- and long-term subsurface water and contaminant transport in the unconfined aquifer at the Hanford Site at several scales. The software will run on desktop computers, scientific workstations, and large computer clusters.

The test procedures apply to all of the software being tested, although tests are limited to representative problems for the class of problems expected to be solved at the Hanford Site to demonstrate applicability for intended use by the CHPRC Integration and Assessments Group.

The MODFLOW calculational software configuration items tested in this STP are:

* **MODFLOW-2000**
* **MODFLOW-2000-MST** (variant of MODFLOW-2000 with features stop dry cells from becoming inactive and provide continuous derivatives)
* **MT3DMS-MST** (variant of MT3DMS with features supporting MODFLOW-2000-MST minimum saturated thickness variant)
* **MODPATH**
* **mod-PATH3DU (calculates particle pathlines on unstructured flow grids using the Waterloo method)**

Supporting software, as identified in CHPRC-00257, *MODFLOW and Related Codes Functional Requirements Document* (Nichols 2009b) (FRD), are not tested in this STP because these were not classified as safety software or graded to a level requiring testing.

Controlled use of this software is managed by CHPRC-00258, *MODFLOW and Related Codes Software Management Plan* (Nichols 2009c) (SMP). The major milestone of the test procedures is issuance of CHPRC-00261, *MODFLOW and Related Codes Acceptance Test Report* (Nichols 2009a) (ATR) that will enable authorization for use for the above software to be granted.

# TEST REQUIREMENTS

## Approach

The general approach for this STP is to test the MODFLOW, MT3DMS, MODPATH, and mod-PATH3DU codes each against test problems specifically chosen with the following attributes: 1) availability of an analytical solution or comparison to [a published] solution to facilitate comparison to a known solution, 2) sufficiently difficult for numerical approximation techniques to resolve that the test will provide not only evidence of a correct solution but a measure of the degree of error in the solution, and 3) ability to substitute Hanford-specific parameter values where possible to facilitative demonstration of applicability for intended use. As such, acceptance criteria necessarily will rely on professional judgment at least in part to evaluate if the solution obtained from the software that implements approximate numerical solution techniques is robust enough compared to the analytical solution or the case replicated to merit acceptance. It is possible to pose easier problems for which the numerical codes will produce exactly the correct solutions, but validation against a difficult-to-resolve problem is more informative. Acceptance criteria are deliberately chosen to avoid problems that arise from comparison of extremely small values that can give large percentage differences but don’t represent any significant difference.

The sequence of testing activities is discussed in the presentation of the test cases in Section 3.3.

## Deliverables

This STP specifies test design, test cases, and test procedures for acceptance and installation testing of MODFLOW and related codes.

For acceptance testing, test results will be documented in an ATR using the format provided in the ATR format guidance referenced in PRC-PRO-IRM-309.

For installation testing, results will be documented in Software *Installation & Checkout Form* (A-6005-149).

## Control Procedures

The test cases in this STP are relatively simple and efficient to conduct and do not require formal tracking or control procedures. The test case logs will be used to document all steps and track results.

## Acceptance Criteria

Acceptance criteria will specify objective numerical tolerances and subjective professional judgment metrics for specific tests that must be met by the code in solving classical groundwater problems with Hanford-specific properties in order to pass. These criteria are specified with the test description in Section 3.3.

## Testing Tasks

The tasks necessary to prepare for and perform testing include code installation (which may require compiling and linking source code using a Fortran compiler, depending on test environment), creating and activating a [code] environment, file transfers, checking input/output files using a text editor program, checking output figures using an image viewer program copying model results from text files using a text editor, and pasting results into Excel spreadsheets used to solve the analytic solutions that provide the basis for validation and compare results.

### Verification & Validation tasks

Tasks necessary to prepare for verification and validation testing are routine with respect to computer usage. MODFLOW and related codes must be installed. Users will run a virus scan of the host computer at completion of the software installation, consistent with requirements of PRC-PRO-IRM-309.

For acceptance testing, the following tasks will occur:

1. Log – the results of test execution, the incidents observed, and any other events pertinent to the test are to be logged on the forms provided as attachments to this STP.
2. Setup – verify that the host computer uses a suitable operating system for MODFLOW and related codes, and that these software are installed, registered as appropriate, and virus-checked. If this software is not installed, complete the installation per directions received from the appropriate provider and virus-check the host computer immediately following software installation.
3. Execution – run the acceptance tests.
4. Evaluation – compare results of the acceptance test cases to the baseline results and evaluate if acceptance criteria are met.
5. Contingencies – in the event that output obtained from the acceptance tests appear flawed, the user may identify and correct errors and restart the test. All such attempts and corrective actions taken will be logged. Return to step 3.
6. Documentation – complete the required documentation of testing in the ATR.
7. Preservation – archive the MODFLOW and related codes software in MKS Integrity™[[1]](#footnote-1) to preserve the baseline as appropriate, along with the model file used for the acceptance test.
8. Review – independent technical review of test results is required and will be documented in the ATR.

For installation testing, the following tasks will occur:

1. Setup – verify that the host computer uses a suitable operating system for the MODFLOW and related codes software, and that software is installed, registered as appropriate, and virus-checked. If the software is not installed, complete the installation and virus-check the host computer immediately following installation.
2. Execution – run the installation tests
3. Evaluation – Compare results of the installation test case to the baseline results and evaluate if acceptance criteria are met.
4. Documentation – complete the required documentation of installation testing.

If software problem(s) (that is, problems with the software itself, not input or other use errors) are identified during testing, a *Problem Report/Change Request* form (A-6005-146) will be prepared by the software tester in accordance with Sections 3.4 of PRC-PRO-IRM-309; the form will document as applicable the following information:

* Nature of required change (Minor/Major)
* Disposition and Proposed Corrective Action
* Impact Analysis
* Affected Hardware components
* Affected Baseline Documentation
* Affected software (e.g., libraries, databases)
* Testing Requirements

Submit the completed *Problem Report/Change Request* form to the software owner who will respond following the process identified in the SMP.

### Responsibilities

The software owner will:

* Conduct acceptance testing or delegate this task to a qualified MODFLOW and related codes software user.
* Assign an independent technical reviewer who is not the person conducting the test to review and approve acceptance test results (the software owner may serve as the independent technical reviewer unless the software owner is also the software user).
* Ensure that acceptance testing results are documented in the ATR, obtain approvals, and issue the ATR.
* Respond to submission of *Problem Report/Change Request* forms as specified in the SMP.
* Maintain HISI entries related to software status, testing, and approval for use of MODFLOW and related codes as identified in PRC-PRO-IRM-309
* Archive a copy of the software and any vendor provided documents in the MKS Integrity™ configuration management system.

The independent technical reviewer will:

* Review this STP and ATR or installation test results for completeness, consistency, clarity and correctness.
* Confirm acceptable test results for acceptance testing.

The software user will do the following before using a software installation to produce results that will be reported in released documents or used for decision making purposes:

* Only use versions of MODFLOW and related codes that are approved for use (following completion of acceptance testing).
* When installing the MODFLOW and related codes, complete the installation test identified in this STP and documents the results using *Software Installation & Checkout Form* (A-6005-149).
* Ensuring that the installation test is repeated and results documented following software or hardware configuration changes to the host computer (e.g., operating system patches or upgrades)

### Risks and Contingencies

No major risks are identified with respect to this test plan. MODFLOW and related codes have a long history of successful application to similar problems as CHPRC intends to use this software to solve and is the most widely used software in the world for this purpose.

# TEST CASES

## Identification

Acceptance test cases will be identified uniquely by the following naming convention:

MF-ATC-#

MT-ATC-#

MP-ATC-#

MU-ATC-#

where MF designates MODFLOW, MT designates MT3DMS, MP designates MODPATH, and MU designates mod-PATH3DU; ATC designates an acceptance test case; and # is the unique test number. Similarly, installation test cases are designated by the following naming convention:

MF-ITC-#, MT-ITC-#, MP-ITC-#, or MU-ITC-#

where ITC designates an installation test case.

## Pass/Fail Criteria

Specific pass/fail criteria for acceptance test cases are identified below in Section 3.3 for each case, and are set to ensure accurate solutions by the numerical solver in the tested software within an objective numerical tolerance. When the software is shown through the testing to meet these criteria, it will be considered to have passed the test.

## Test Cases

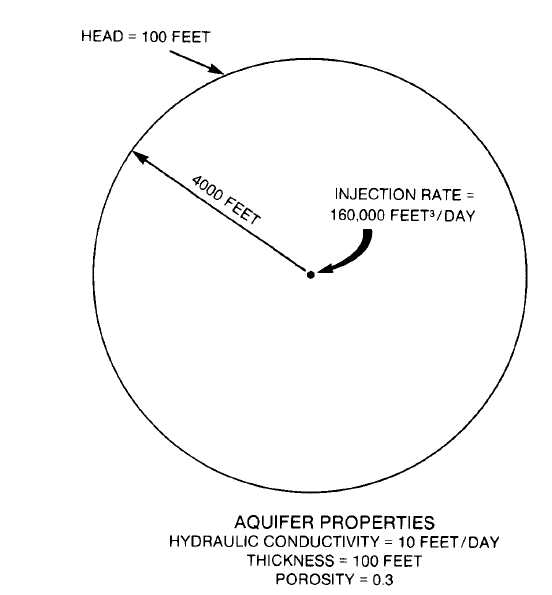
Two acceptance test cases and two installation test cases, one each for MODFLOW and MT3DMS, are detailed below with acceptance criteria and expected results for each. The MODFLOW test is applicable to both the baseline and variant versions of MODFLOW; testing for each will be conducted and documented separately.

For MODPATH, four test cases and one installation case are detailed below with acceptance criteria and expected results for each. For modPATH-3DU, two test cases and one installation case are detailed below. All six of these tests are executed via a batch file, runme.bat, which then outputs the results of the tests to “All\_tc\_results.xlsx”, a document which contains the pass/fail status of each test.

### MP-ATC-1: Forward Particle Tracking from an Injection Well

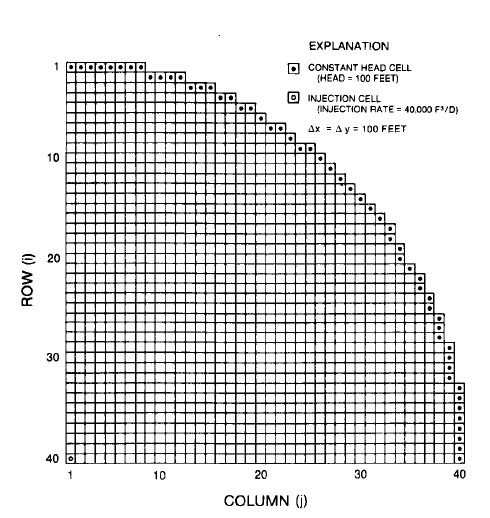
#### Test Case Description

MP-ATC-1 tests MODPATH’s ability to repeat within acceptable tolerance levels a forward-particle tracking test conducted in Pollock, 1988, *Semianalytical Computation of Path Lines for Finite-Difference Models*. The test in Pollock, 1998, involves forward particle tracking in a steady-state system with an injection well. A well injects water at a steady state into a confined aquifer. Around the well in a circle, heads are held constant. This setup is shown in Figure 3‑1. This system is symmetrical, so only one-quarter of the circular flow field needs to be calculated for this test. The flow model setup in Pollock, 1988, is shown in Figure 3‑2. Ten particles, equally spaced apart from each other, were placed in an arc around the well. These particles were tracked forward, and their traveled distances at 2,500, 5,000, and 7,500 days are shown in Figure 3‑3. MODPATH’s ability to repeat the results in Figure 3‑3 is the pass/fail metric this test case is based upon.



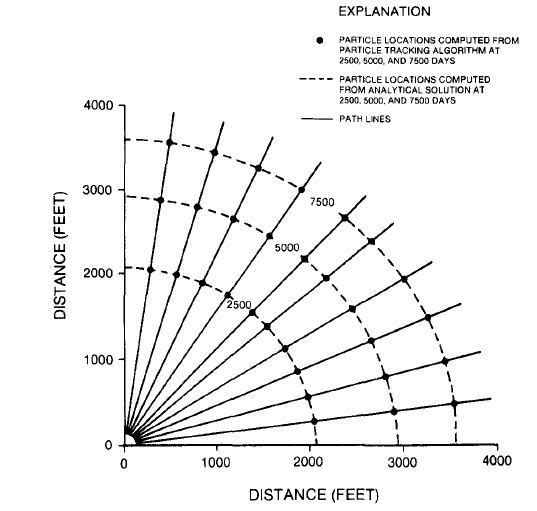
Source: Pollock, 1988

Figure 3‑1. MP-ATC-1 Layout



Source: Pollock, 1988

Figure 3‑2. MP-ATC-1 MODFLOW Setup



Source: Pollock, 1988

Figure 3‑3. Particle Location Over Time in MP-ATC-1

#### Test Case Setup

Test setup consists of four parts:

* Assemble the MODFLOW model to serve as the underlying flow model. Use the inputs stated in Pollock, 1988, and estimate inputs when necessary.
* Assemble the MODPATH model for particle tracking. Use the inputs stated in Pollock, 1988, and estimate inputs when necessary.
* Digitize Figure 3‑3 to determine the locations of the points during the times of interest.
* Assess the pass/fail status of the test by comparing the MODPATH results to the digitized results of Figure 3‑3.

##### Assemble the MODFLOW model

The MODFLOW model was assembled using the values in Pollock, 1988, when provided and made reasonable assumptions at values needed, but not provided by Pollock, 1988. Model inputs are seen in Table 3‑1. The model has a single layer and has 40 rows and 40 columns each with a length and width of 30.48 m (100 ft). The thickness of the model is set to a uniform 30.48 m (100 ft). Constant head cells were assigned to match the constant head boundary cells in Figure 3‑2, and have a constant head of 30.48 m (100 ft). Constant head cell locations are listed Table 3‑2. The injection well is located in the bottom left corner (row 40, column 1) and injects at a rate of 1,133 m3/day (40,000 ft3/day), representing a quarter of the pumping rate of the full-size model. The center of the well is located in the center of the cell.

| Table 3‑1. MODFLOW Model Parameter Values for MP-ATC-1 | | | |
| --- | --- | --- | --- |
| Variable name | Variable Value | Units | Source |
| Number of rows | 40 | N/A | Pollock, 1988, Figure 6 |
| Number of columns | 40 | N/A | Pollock, 1988, Figure 6 |
| Height of rows | 30.48 (100) | m (ft) | Pollock, 1988, Figure 6 |
| Width of columns | 30.48 (100) | m (ft) | Pollock, 1988, Figure 6 |
| Number of layers | 1 | N/A | Assumed |
| Thickness of layer | 30.48 (100) | m (ft) | Pollock, 1988 |
| Injection rate | 1,133 (40,000) | m3/day (ft3/day) | Pollock, 1988, Figure 5 |
| Hydraulic conductivity (hk and vka) | 3 (10) | m/day (ft/day) | Pollock, 1988, Figure 5 for hk, vka assumed |
| Constant head | 30.48 (100) | m (ft) | Pollock, 1988, Figure 6 |
| Starting head | 30.48 (100) | m (ft) | Assumed |
| Number of stress periods | 15 | N/A | Assumed |
| Stress period length | 500 | days | Assumed |
|  | | | |

| Table 3‑2. Constant Head Boundary Cell Locations | | | | | | | | | | |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Constant Head Boundary Cells | |  | Constant Head Boundary Cells | |  | Constant Head Boundary Cells | |  | Constant Head Boundary Cells | |
| Row | Column |  | Row | Column |  | Row | Column |  | Row | Column |
| 1 | 1 |  | 3 | 15 |  | 13 | 29 |  | 27 | 38 |
| 1 | 2 |  | 4 | 16 |  | 14 | 30 |  | 28 | 38 |
| 1 | 3 |  | 4 | 17 |  | 15 | 31 |  | 29 | 39 |
| 1 | 4 |  | 5 | 18 |  | 16 | 32 |  | 30 | 39 |
| 1 | 5 |  | 5 | 19 |  | 17 | 33 |  | 31 | 39 |
| 1 | 6 |  | 6 | 20 |  | 18 | 33 |  | 32 | 39 |
| 1 | 7 |  | 7 | 21 |  | 19 | 34 |  | 33 | 40 |
| 1 | 8 |  | 7 | 22 |  | 20 | 34 |  | 34 | 40 |
| 2 | 9 |  | 8 | 23 |  | 21 | 35 |  | 35 | 40 |
| 2 | 10 |  | 9 | 24 |  | 22 | 36 |  | 36 | 40 |
| 2 | 11 |  | 9 | 25 |  | 23 | 36 |  | 37 | 40 |
| 2 | 12 |  | 10 | 26 |  | 24 | 37 |  | 38 | 40 |
| 3 | 13 |  | 11 | 27 |  | 25 | 37 |  | 39 | 40 |
| 3 | 14 |  | 12 | 28 |  | 26 | 38 |  | 40 | 40 |

##### Assemble the MODPATH model

Setup for the MODPATH model required defining the locations of the particles, as well as the porosity. Pollock, 1988 states that the porosity is 0.3. Ten particles were used for forward tracking in Pollock, 1988, which describes the particle placement as “at a radial distance of 150 feet from the center of the well.” Because the MODFLOW Well Package designates a well as the entire cell the well is in, this was interpreted to mean the distance is measured from the center of the cell the well is in. Therefore, starting particle locations were placed evenly-spaced in an arc with a 150-foot radius from the center of the well cell (Table 3‑3). These locations were calculated using a python script, which will be discussed in Section 3.3.1.5.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Table 3‑3. Particle Starting Locations | | | | | | |
| Particle ID | Row | Column | Local X | Local Y | Local Z | Release Time |
| 1 | 40 | 2 | 1 | 0.51 | 0.5 | 0 |
| 2 | 40 | 2 | 0.9596 | 0.8559 | 0.5 | 0 |
| 3 | 39 | 2 | 0.8404 | 0.1832 | 0.5 | 0 |
| 4 | 39 | 2 | 0.6491 | 0.4742 | 0.5 | 0 |
| 5 | 39 | 2 | 0.3957 | 0.7132 | 0.5 | 0 |
| 6 | 39 | 2 | 0.0941 | 0.8873 | 0.5 | 0 |
| 7 | 39 | 1 | 0.7605 | 0.9872 | 0.5 | 0 |
| 8 | 39 | 1 | 0.4128 | 1.0075 | 0.5 | 0 |
| 9 | 39 | 1 | 0.0698 | 0.947 | 0.5 | 0 |
| 10 | 40 | 2 | 0.9596 | 0.1641 | 0.5 | 0 |

##### Digitize the Particle Tracks

The particle tracks were digitized in order to compare the results of the MODPATH model to those in Pollock, 1988. First, the image of Figure 3‑3 was captured and saved. Then, the image was digitized using WebPlotDigitizer, an open-source software. Finally, the locations and travel distances of the particles at each of the times was interest were digitized and saved into a comma-separated file. The data in this file is the metric against which one of the pass/fail criteria is calculated.

##### Pass/Fail Criteria

The acceptance criteria for this test are as follows:

* Criterion 1 – the MODPATH simulation produces straight particle tracks that radiate outward
* Criterion 2 – the percent difference between the length of the flow paths digitized from Figure 3‑3 calculated value must not be more than 5%. The length of the flow paths calculated by MODPATH are calculated in post-processing by selecting the global X and Y values for each particle at the time of interest, and calculating the distance from that particle to the lower left corner of the model.

Criterion 1 gives evidence that the particle tracks are moving according to the flow direction. Criterion 2 gives evidence that the particles are moving at a speed that is within an acceptable range of similarity to the particles in Pollock, 1988. Criterion 1 must be determined using professional judgment, by observing the image files to confirm that the particle tracks radiate outward, as seen in Figure 3‑3.

#### Sources of Error

There are several sources of error in this test case. The first is that a different version of MODFLOW was used to calculate the underlying flow model in Pollock, 1988 than was used in this test case. The second is that the particles were calculated using a method very similar to that used by MODPATH, but did not use the version of MODPATH tested in this document. The third is that the locations of the points at 0, 2,500, 5,000, and 7,500 days were not explicitly stated and had to be reproduced via digitization. Errors may have been introduced in the reproduction, either through the calculation of the location of the starting points, or through minor errors in the digitization of Figure 3‑3.

#### File Structure

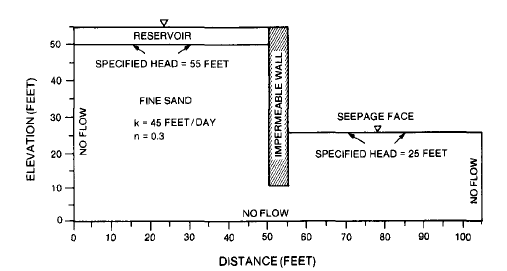
All files for MP-ATC-1 are contained within the “Test\_Case\_1” folder in the root directory. The structure within that folder is as follows:

* /gw\_codes (This folder contains the executables used in the test case)
  + mf2k-chprc08spl.exe
    - Description: executable of single-precision MODFLOW, “CHPRC Build 8”. Used in S01\_tc1.py to execute the MODFLOW model.
  + mp6.exe
    - Description: executable of MODPATH, version 6. Used in S01\_tc1.py to execute the MODPATH model.
* /output (This folder contains the post-processing files used to determine the pass/fail status of the test case)
  + /figures (This folder contains figures showing the results of the MODPATH forward particle tracking at 2,500, 5,000, and 7,500 days)
    - 2500\_days.png
      * Description: image of the MODPATH forward particle tracking result at day 2,500. Created by S01\_tc1.py. Used to determine the pass/fail status of Criterion 1.
    - 5000\_days.png
      * Description: image of the MODPATH forward particle tracking result at day 5,000. Created by S01\_tc1.py. Used to determine the pass/fail status of Criterion 1.
    - 7500\_days.png
      * Description: image of the MODPATH forward particle tracking result at day 7,500. Created by S01\_tc1.py. Used to determine the pass/fail status of Criterion 1.
  + tc1\_results.csv
    - Description: This file contains the pass/fail results for Criterion 2. The pass/fail results are listed in column E, and columns A-D contain the information used to determine the pass/fail result.
* /preprocessing (This folder contains data used in model calculation or post-processing. These data are static and do not need to be re-calculated every time the model is run.)
  + chb\_t1.csv
    - Description: This file contains the row, column, and head data of the constant head cells. Row and column data of the constant head cells are copied from Figure 3‑2.
  + figure\_7\_distances.csv
    - Description: This file contains the location data digitized from Figure 3‑3. These location data are used as the basis against which the MODFLOW particle tracks are compared for Criterion 2 of the pass/fail criteria.
* /workspace (This folder is empty before the test cases are run, but will be populated with all the MODFLOW and MODPATH files used in the test case).
  + Many of the test files which will be populated here each are titled “test\_case\_1”, and end with the following file types, listed in alphabetical order: BAS, CHD, DIS, LPF, NAM, OC, PCG, WEL, CBC, GLO, LIST, HDS, MPBAS, MPNAM, MPSIM, MPEND, MPLST, MPPTH
  + starting\_locs.loc
    - Description: this is the file of starting location points. It must match Table 3‑3 for the data present in both.
  + MPATH6.LOG
    - Description: This is a log file created by MODPATH.
* runme.bat
  + Description: A batch file which executes “S01\_tc1.py”. Called by the runme.bat file in the root directory.
* S01\_tc1.py
  + Description: A python script that creates the files for the MODFLOW and MODPATH models, executes the models, post-processes the results, and prints the pass/fail status of the test to “tc1\_results.csv” in /output.
* Write\_starting\_locations.py
  + Description: calculates the locations of the starting point files.

### MP-ATC-2: Particle Tracking in Non-Uniform Flow

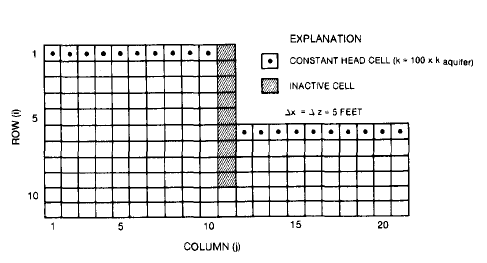
#### Test Case Description

MP-ATC-2 tests MODPATH’s ability to repeat within acceptable tolerance levels a test conducted in Pollock, 1988 on forward-particle tracking of a non-uniform flow field. This test in Pollock, 1988 involves examining flow under an impermeable wall in the steady-state system shown in Figure 3‑4. To the left of an impermeable retaining wall is a 50-foot thickness of fine sand overlain by 1.5 m (5 ft) of water in a reservoir. A seepage face at an elevation of 7.6 m (25 ft) above the base of the aquifer is present to the right of the retaining wall. The flow model setup in Pollock, 1988 is shown in Figure 3‑5. Particles were released at the base of the reservoir and tracked forward until they reached the seepage face, as shown in Figure 3‑6. MODPATH’s ability to repeat the results in Figure 3‑6 is the pass/fail metric this test case is based upon.



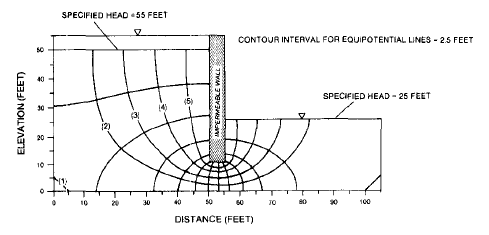
Source: Pollock, 1988

Figure 3‑4. MP-ATC-2 Layout



Source: Pollock, 1988

Figure 3‑5. MP-ATC-2 MODFLOW Layout



Source: Pollock, 1988

Figure 3‑6. Particle Location Over Time in MP-ATC-2

#### Test Case Setup

Test setup consists of four parts:

* Assemble the MODFLOW model to serve as the underlying flow model. Use the inputs stated in Pollock, 1988, and estimate inputs when necessary.
* Assemble the MODPATH model for particle tracking. Use the inputs stated in Pollock, 1988, and estimate inputs when necessary.
* Digitize Figure 3‑6 to determine the particles’ ending locations and pathlines.
* Assess the pass/fail status of the test by comparing the MODPATH results to the digitized results of Figure 3‑6.

##### Assemble the MODFLOW Model

The MODFLOW model was assembled using the values in Pollock, 1988, when provided and made reasonable assumptions at values needed, but not provided by Pollock, 1988. Model inputs are seen in Table 3‑4. This model has a single layer, with 11 rows and 21 columns, each with a length and width of 1.5 m (5 ft). The thickness of the model is set to a uniform 7.6 m (25 ft). The thickness was not defined in Pollock, 1988, so a thickness of 7.6 m (25 ft) was assumed. No-flow cells were assigned as seen in Figure 3‑5. Constant heads of 16.8 m (55 ft) and 7.6 m (25 ft) were assigned to the cells representing the reservoir and seepage face, respectively, as seen in Figure 3‑5. Starting heads were also not listed in Pollock, 1998, so it was assumed that the area beneath the reservoir and the impermeable berm had a starting head of 16.8 m (55 ft), and the area beneath the seepage face had a starting head of 7.6 m (25 ft).

| Table 3‑4. MODFLOW Model Parameter Values for MP-ATC-2 | | | |
| --- | --- | --- | --- |
| Variable name | Variable value | Units | Source |
| Number of rows | 11 | N/A | Pollock, 1988, Figure 9 |
| Number of columns | 21 | N/A | Pollock, 1988, Figure 9 |
| Height of rows | 5 | ft | Pollock, 1988, Figure 9 |
| Width of columns | 5 | ft | Pollock, 1988, Figure 9 |
| Number of layers | 1 | N/A | Assumed |
| Thickness of layer | 7.6 (25) | m (ft) | Assumed |
| Hydraulic conductivity (aquifer, hk and vka) | 13.7 (45) | m/day (ft/day) | Pollock, 1988, Figure 8 for hk, vka assumed |
| Hydraulic conductivity (reservoir and seepage face, hk and vka) | 1,372 (4,500) | m/day (ft/day) | Pollock, 1988, Figure 9 for hk, vka assumed |
| Constant head (reservoir) | 16.8 (55) | m (ft) | Pollock, 1988, Figure 8 |
| Constant head (seepage face) | 7.6 (25) | m (ft) | Pollock, 1988, Figure 8 |
| Starting head (columns 1 through 11) | 16.8 (55) | m (ft) | Assumed |
| Starting head (columns 12 through 21) | 7.6 (25) | m (ft) | Assumed |
| Number of stress periods | 30 | N/A | Assumed |
| Stress period length | 1 | days | Assumed |

##### Assemble the MODPATH Model

Setup for the MODPATH model required defining the locations of the particles, as well as the porosity. Pollock, 1988 states that the porosity is 0.3. Five particles were used for forward tracking in Pollock, 1988. The particle track locations were estimated for use in the MODPATH model and listed in Table 3‑5. Particle 1 was not modeled, as its starting location was unclear.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Table 3‑5. Particle Starting Locations, MP-ATC-2 | | | | | | | | |
| Particle ID | Grid | Layer | Row | Column | Local X | Local Y | Local Z | Release Time |
| 2 | 1 | 1 | 1 | 3 | 0.5 | 0 | 0.5 | 0 |
| 3 | 1 | 1 | 1 | 5 | 0.5 | 0 | 0.5 | 0 |
| 4 | 1 | 1 | 1 | 7 | 0.5 | 0 | 0.5 | 0 |
| 5 | 1 | 1 | 1 | 9 | 0.5 | 0 | 0.5 | 0 |

##### Digitize the Particle Tracks

The particle tracks were digitized in order to compare the results of the MODPATH model to those in Pollock, 1988. First, the image of Figure 3‑6 was captured and saved. Then, that image file was converted into a raster and given arbitrary projection information. Finally, the particle pathlines were digitized in a GIS program and saved as a shapefile. The endpoints of the particle pathlines were also digitized in a GIS program and saved as a shapefile. The data in these shapefiles are the metric against which the pass/fail criteria are calculated.

##### Pass/Fail Criteria

The acceptance criteria for this test are as follows:

* Criterion 1 – the MODPATH simulation produces particle tracks that are visually similar to those seen in Figure 3‑6, according to professional judgment.
* Criterion 2 – the percent difference between the particle end points digitized from Figure 3‑6 and the MODPATH-calculated particle end points must not be more than 10%.

Criterion 1 gives evidence that the particle tracks are moving according to the flow direction. Criterion 2 gives evidence that the particles’ ending locations are within an acceptable range of similarity to the particles in Pollock, 1988. Criterion 1 must be determined using professional judgment, by observing the output image file to confirm that the particle tracks follow pathlines similar to those seen in Figure 3‑6. The pass/fail status of Criterion 2 will be printed to a file, listed in Section 3.3.2.5.

##### Sources of Error

There are several sources of error in this test case. The first is that a different version of MODFLOW was used to calculate the underlying flow model. The second is that the particles were calculated using a method very similar to that used by MODPATH, but did not use the version of MODPATH tested in this document. The third is that Figure 3‑6 as it was printed in Pollock, 1988 was slightly warped and required georeferencing to reduce the effect on the pathline shape. Some effect of the warped figure may still remain on the digitized pathlines, causing a slightly different shape than the true results.

#### File Structure

All files for MP-ATC-2 are contained within the “Test\_Case\_2” folder in the root directory. The structure within that folder is as follows:

* /output (This folder contains the post-processing files used to determine the pass/fail status of the test case)
  + Compared\_pathlines.png
    - Description: image comparing the pathlines digitized from Figure 3‑6 (“Digitized Pathlines”) to those created for this test case (“Modpath6 Pathlines”). Created by S01\_tc2.py. Used to determine the pass/fail status of Criterion 1.
  + tc2\_results.csv
    - Description: This file contains the pass/fail results for Criterion 2. The pass/fail results are listed in columns J and K, and columns A-I contain the information used to determine the pass/fail result.
* /preprocessing (This folder contains data used in model calculation or post-processing. These data are static and do not need to be re-calculated every time the model is run.)
  + /digitize (This folder contains the digitized shapefiles of the particle tracks and the particle endpoints, as seen in Figure 3‑6)
    - endpoints.shp and related files
      * Description: Approximate ending location of the particle pathlines in Figure 3‑6.
    - figure\_10\_pathline.shp and related files
      * Description: Particle pathlines digitized from a raster of Figure 3‑6.
  + /gwpath\_images (This folder contains images copied from Pollock, 1988)
    - figure\_10\_pathline.png
      * Description: An image file of Figure 3‑6. This was captured from a digital version of Pollock, 1988 using a screen-capture tool.
  + /gwpath\_rasters (This folder contains the rasters created from the images in /gwpath\_images)
    - figure\_10\_pathline.tif and associated aux file
      * Description: The raster of “figure\_10\_pathline.png” created by “S00\_pngs\_2\_tiffs.py”.
    - figure\_10\_pathline.tif.points
      * Description: the points used to digitize the raster of the image in order to remove the warp.
    - Figure\_10\_referenced and associated aux file
      * Description: A georeferenced version of “figure\_10\_pathline.tif”. It was georeferenced in QGIS using a transformation type of Polynomial 1 and nearest neighbor resampling. The points used in the georeferencing are saved in “figure\_10\_pathline.tif”.
    - Starting\_location.shp and related files
      * A point file which defines the arbitrarily-selected location of the upper-left corner of the figures during the digitization process.
  + particle\_starting\_locs\_ex2.csv
    - Description: this is the file of starting location points. It must match Table 3‑5 for the data present in both.
  + S00\_pngs\_2\_tiffs.py
    - Description: This python script digitizes an image and assigns it an arbitrary projection. This is done so the particle locations can be defined and compared to the outcomes of this test.
* /workspace (This folder is empty before the test cases are run, but will be populated with all the MODFLOW and MODPATH files used in the test case).
  + Many of the test files which will be populated here each are titled “test\_case\_2”, and end with the following file types, listed in alphabetical order: BAS, CHD, DIS, LPF, NAM, OC, PCG, WEL, CBC, GLO, LIST, HDS, MPBAS, MPNAM, MPSIM, MPEND, MPLST, MPPTH
  + starting\_locs\_ex2.loc
    - Description: this is the file of starting location points. It must match Table 3‑5 for the data present in both.
  + MPATH6.LOG
    - Description: This is a log file created by MODPATH.
* runme.bat
  + Description: A batch file which executes S01\_tc2.py. Called by the runme.bat file in the root directory.
* S01\_tc2.py
  + Description: A python script that creates the files for the MODFLOW and MODPATH models, executes the models, post-processes the results, and prints the pass/fail status of the test to “tc2\_results.csv” in /output.
* texas\_gam.prj
  + Description: projection data for the projection arbitrarily selected for use in this test case.
* Write\_starting\_locations.py
  + Description: calculates the locations of the starting point files.

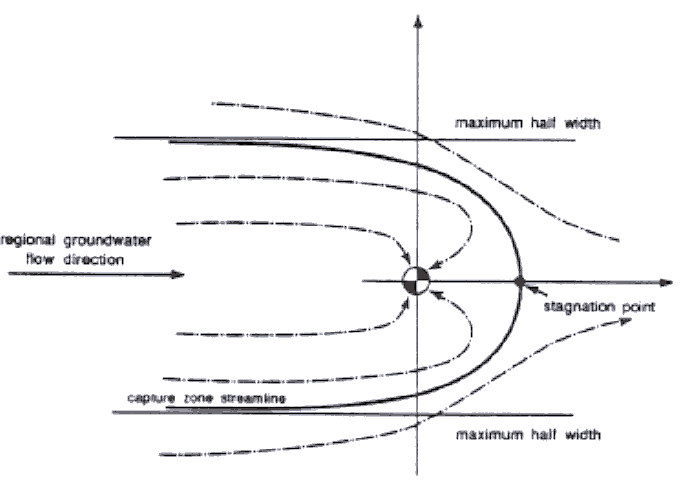
### MP-ATC-3: Capture Zone in an Unconfined Aquifer

#### Test Case Description

MODPATH’s reverse particle tracking capabilities are commonly used to map capture zones in an unconfined aquifer at the Hanford Site. In this test, results from a MODPATH reverse particle tracking simulation are compared to an analytically-calculated capture zone. The analytical solution (Grubb, 1993, *Analytical Model for Estimation of Steady-State Capture Zones of Pumping Wells in Confined and Unconfined Aquifers*) calculates the shape of a capture zone with the following conditions:

* The aquifer is homogeneous, isotropic, and infinite in horizontal extent.
* The flow conditions are uniform and steady-state.
* The unconfined aquifer has a horizontal lower confining layer with no leakage, rainfall infiltration, or other vertical recharge.
* The specific yield of the aquifer is neglected.
* Vertical gradients are negligible.
* The pumping well is fully penetrating, open over the thickness of the aquifer, and pumps at a constant rate.

Taking all these assumptions into account, a well pumping at a constant rate will produce a capture zone extend infinitely in the upgradient direction and end in the downgradient direction, as shown in Figure 3‑7. The maximum width of the upgradient capture zone as measured from the center of the well (ymax­) and the stagnation point, the distance from the pumping well to the down-gradient edge of the capture zone (the stagnation point, or *x0*), can be calculated analytically.



Source: Yang, Spencer, and Gates, 1995, *Analytical Solutions for Determination of Non-Steady-State and Steady-State Capture*

Figure 3‑7. Capture zone in an unconfined aquifer

The maximum width of a capture zone an unconfined aquifer is defined by the following equation from Grubb (1993):

where:

*ymax* = the maximum width of the capture zone, where y0 intersects the center of the well

*Q* = the pumping rate

*L* = the distance between *h1* and *h2*

*K* = the hydraulic conductivity

*h1* = the upgradient head

*h2* = the downgradient head

The position of the stagnation point is calculated using the following equation:

where:

*x0* = the stagnation point

*Q* = the pumping rate

*L* = the distance between *h1* and *h2*

*K* = the hydraulic conductivity

*h1* = the upgradient head

*h2* = the downgradient head

MODPATH’s ability to recreate the *ymax* and *x0* within an acceptable tolerance level is the pass/fail metric this test case is based upon.

#### Test Case Setup

Setting up the test consisted of four parts:

* Set up the analytical calculation.
* Assemble the MODFLOW model to serve as the underlying flow model. Use the inputs from the analytical calculation.
* Assemble the MODPATH model for particle tracking.
* Execute the MODFLOW and MODPATH models and calculate the analytical solution.
* Assess the pass/fail status of the test by comparing the MODPATH results to the analytical results.

##### Analytical Calculation Setup

The analytical solutions for *ymax* and *x0* were set up according to the equations listed in Section 3.3.3.1. The values used to calculate the analytical solution are shown in Table 3‑5. The extraction rate (Q) used is a value similar to those use in remediation at the Hanford Site, the hydraulic conductivity (K) falls within the range of the K seen in the Ringold Wooded Island Formation Member unit E (CP-47631, *Model Package Report: Central Plateau Groundwater Model*), and the gradient also falls within the range of gradients seen at the Hanford Site (ECF-Hanford-17-0241, *Hydraulic Gradient and Velocity Calculations for RCRA Sites in 2017*).

| Table 3‑5. Analytical Solution Parameter Values for MP-ATC-3 | | |
| --- | --- | --- |
| Variable name | Variable Value | Units |
| Extraction rate (Q) | 545 (19,455) | m3/day (ft3/day) |
| Hydraulic conductivity (K) | 304.8 (1000) | m/day (ft/day) |
| h1 head (h1) | 60.96 (200) | m (ft) |
| h2 head (h2) | 60.67 (199.048) | m (ft) |
| Distance between h1 and h2 (L) | 24,384 (80,000) | m (ft) |

##### Assemble the MODFLOW Model

The MODFLOW model was assembled to reflect the analytical solution’s requirements and use the same values used in the analytical solution, shown in Table 3‑5. Other values required in the setup of the MODFLOW model are shown in Table 3‑6. The MODFLOW model has one 60.96-m (200-ft) thick layer and is 24,384 m (80,000 ft) long in the x direction, and 12,192 m (40,000 ft) long in the y direction. It is unconfined. The right and left boundaries are each constant head boundaries to simulate h­1 and h2, respectively, in the analytical solution. These boundaries are assigned the same h­1 and h2 values as the analytic solution. The distance between these boundaries, the L in the analytical solution, is the length of the model in the x-direction. The well is placed at the halfway point in the y direction, and two-thirds of the way to the right in the x-direction. This was done to avoid boundary effects.

| Table 3‑6. MODFLOW Parameter Values for MP-ATC-3 | | |
| --- | --- | --- |
| **Variable name** | **Variable Value** | **Units** |
| Pumping well location | row 401, column 1067 | N/A |
| Constant head (left) | 60.96 (200) | m (ft) |
| Constant head (right) | 60.67 (199.048) | m (ft) |
| Number of layers | 1 | N/A |
| Starting head | 60.96 (200) | m (ft) |

Listed below are the analytical solution’s requirements and how the MODFLOW model addressed those requirements:

* Requirement: The aquifer is homogeneous, isotropic, and infinite in horizontal extent.
  + Addressed: The aquifer’s vertical and horizontal hydraulic conductivities are constant through the model and equal each other. Though the nature of finite-difference grid modeling does not allow for infinite extents, the grid was made to extend for a long distance in the X and Y directions, to minimize boundary effects.
* Requirement: The flow conditions are uniform and steady-state.
  + Addressed: No variations are present in the constant head boundaries or well extraction rate. The model was set up as a steady-state model.
* Requirement: The unconfined aquifer has a horizontal lower confining layer with no leakage, rainfall infiltration, or other vertical recharge.
  + Addressed: MODFLOW requires that the bottom layer of any model behave as though it overlies a horizontal confining layer with no vertical recharge.
* Requirement: The specific yield of the aquifer is neglected.
  + Addressed: Specific yield is only calculated for transient solutions, and this is a steady-state solution.
* Requirement: Vertical gradients are negligible.
* Requirement: The pumping well is fully penetrating, open over the thickness of the aquifer, and pumps at a constant rate.
  + Addressed: This model uses the Well Package, which assumes wells cover the length of the cell they’re in. This model has only one layer, which is the aquifer, so the well is fully penetrating and open over the thickness of the model. The well is set up to pump at a constant rate.

##### Assemble the MODPATH Model

Setup for the MODPATH model required defining the locations of the particles, as well as the porosity. The porosity was set to 0.3. The particle placement was chosen to highlight the largest possible capture zone defined by reverse particle tracking. Two particles were seeded at the right boundary of the well cell, one at 49.9% and one at 50.1% of the cell length in the y direction. In the z direction, the particles were both seeded at 50% of the cell height. Because the hydraulic gradient goes from left to right, particles placed at the right side of the cell will capture the stagnation in the x direction. As particles are placed closer to the center, the path traveled to get to those points get closer to the *ymax* and *x0* of the analytical solution. The particles for this test case were placed as close to the center as possible, while still resulting in unique particle paths.

##### Execute the Models and Calculate the Analytical Solution

The MODFLOW and MODPATH models were assembled and executed using a python script. That script is discussed further in Section 3.3.3.5. The analytical solution was calculated using the same script.

##### Pass/Fail Criteria

The acceptance criteria for this test are as follows:

* Criterion 1 – The MODPATH simulation produces a *ymax* value within 10% of the analytical *ymax* value.
* Criterion 2 – The MODPATH simulation produces a *x0* value within 10% of the analytical *x0* value.

These criteria ensure that the MODPATH simulation is performing within an acceptable tolerance of the analytical solution.

#### Sources of Error

There are several sources of error in this test case. The first is that an infinite model can never be truly reproduced with a finite-difference model. This was addressed by making the model much larger than the *ymax* and *x0* of the analytical solution. Another source of error is the way the particle tracks are calculated by MODPATH. MODPATH calculates particle movement from cell face to cell face, therefore, curves in the analytical solution will not be perfectly mimicked.

One source of error in this test case is that the maximum y extent on the southern particle track is slightly less than the maximum y extent on the northern particle track. The reason for this is unclear.

#### File Structure

All files for MP-ATC-3 are contained within the “Test\_Case\_3” folder in the root directory. The structure within that folder is as follows:

* /gw\_codes (This folder contains the executables used in the test case)
  + mf2k-chprc08spl.exe
    - Description: executable of single-precision MODFLOW, “CHPRC Build 8”. Used in S01\_tc1.py to execute the MODFLOW model.
  + mp6.exe
    - Description: executable of MODPATH, version 6. Used in S01\_tc1.py to execute the MODPATH model.
* /output (This folder contains the post-processing files used to determine the pass/fail status of the test case)
  + backwards.png
    - Description: image comparing the analytical solution to the MODPATH pathlines, cropped to show only the are of interest, not the full model.
  + tc3\_results.csv
    - Description: This file contains the pass/fail results for both the pass/fail criteria. The pass/fail results are listed in columns D, H, and K. The remaining columns contain the information used to determine the pass/fail results.
* /workspace (This folder is empty before the test cases are run, but will be populated with all the MODFLOW and MODPATH files used in the test case).
  + Many of the test files which will be populated here each are titled “test\_case\_3”, and end with the following file types, listed in alphabetical order: BAS, CHD, DIS, LPF, NAM, OC, PCG, WEL, CBC, GLO, LIST, HDS, MPBAS, MPNAM, MPSIM, MPEND, MPLST, MPPTH
  + starting\_pts.loc
    - Description: this is the file of starting location points. The starting locations must match the description in Section 3.3.3.2.3.
  + MPATH6.LOG
    - Description: This is a log file created by MODPATH.
* fetter.py
  + Description: This python script defines the equations used to calculate the analytical solutions.
* particle\_starting\_locs\_backwards.csv
  + Description: this file contains the starting location data for the particles and is used to create “starting\_pts.loc”.
* runme.bat
  + Description: A batch file which executes “S01\_tc3.py” and “S02\_pp\_tc3.py”. Called by the runme.bat file in the root directory.
* S01\_tc3.py
  + Description: A python script that creates the files for the MODFLOW and MODPATH models, executes the models, and calculates the analytical results. It does some post-processing by creating creates the “backwards.png” file in /output.
* S02\_pp\_tc3.py
  + Post-processes the results and prints the pass/fail status of the test to “tc3\_results.csv” in /output.

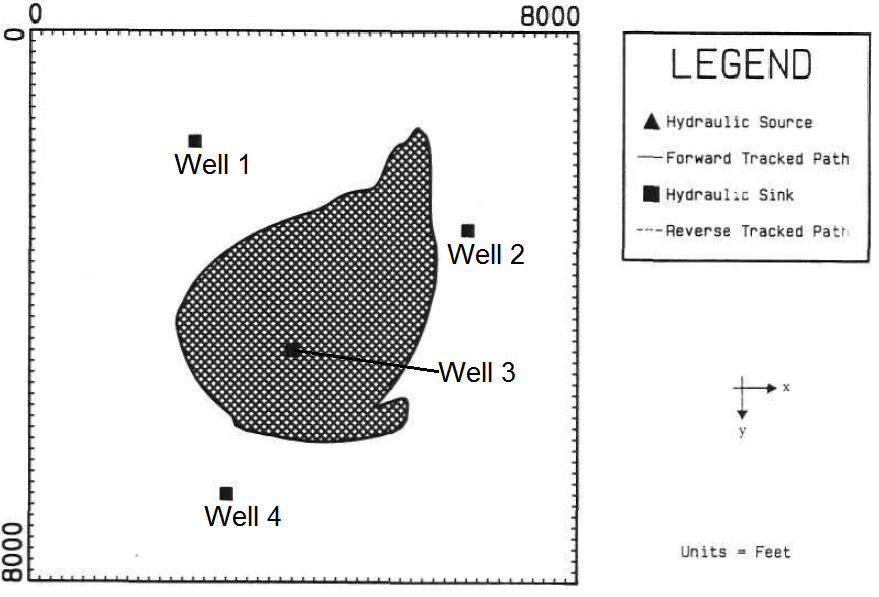
### MP-ATC-4 and MP-ITC-1: Capture Zone in a Heterogeneous Aquifer

#### Test Case Description

MP-ATC-4 (which is the same as MP-ITC-1) tests MODPATH’s ability to recreate within acceptable tolerance levels a ten-year capture zone in a heterogeneous aquifer. The capture zone recreated by this test was calculated in ISWS/BUL-69/87, *GWPATH: Interactive Ground-Water Flow Path Analysis*. The test in ISWS/BUL-69/87 defines a ten-year capture zone of an extraction well (shown in Figure 3‑8) in an aquifer with heterogeneous hydraulic conductivity (shown in Figure 3‑9), and with several other active extraction wells operating nearby (shown in Figure 3‑8). MODPATH’s ability to produce a 10-year capture zone within acceptable tolerance levels of the one shown in Figure 3‑8 is the pass/fail metric this test case is based upon.

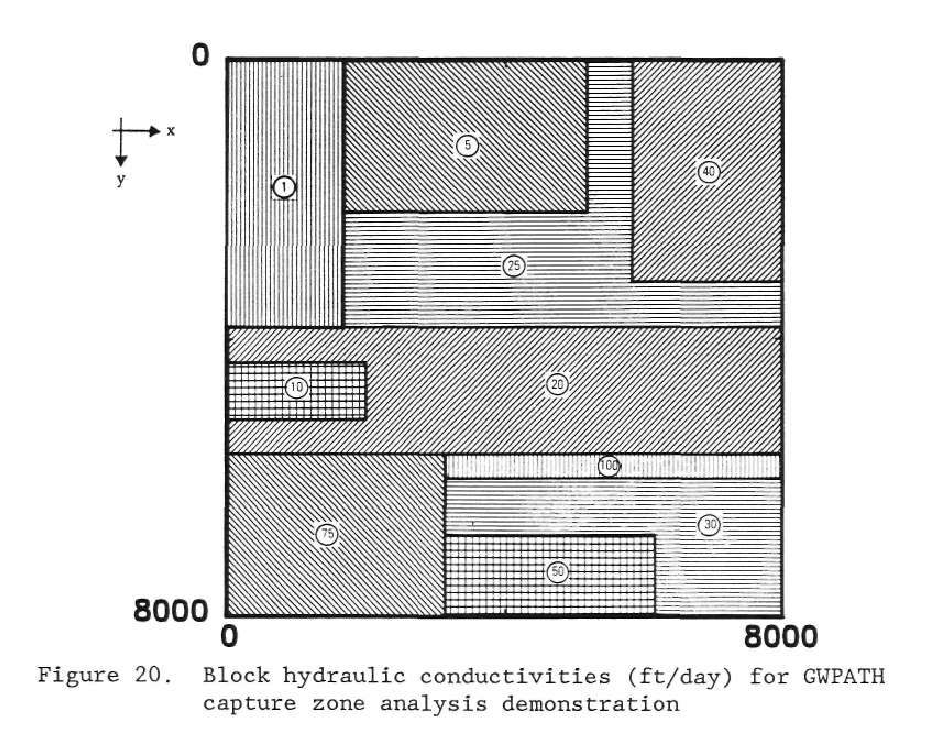
The test setup for flow in ISWS/BUL-69/87 requires extraction wells, constant head boundaries, and a variable hydraulic conductivity field. The variable hydraulic conductivity field is shown in Figure 3‑9. The extraction wells shown in Figure 3‑8 have the coordinates and pumping rates shown in Table 3‑8. The boundary types of the flow model are not explicitly stated by ISWS/BUL-69/87; very little information about the flow model is given at all, including how the flow field was calculated. However, by investigating Figure 3‑10, it can be safely assumed that all boundaries are constant head boundaries. The heads of the top and bottom boundaries are explicitly listed in Figure 3‑10 as 30.48 (100) and 18.29 (60) m (ft), respectively. The right and left boundaries appear to represent a linear stepdown in heads from 30.48 (100) to 18.29 (60) m (ft).

The setup for particle tracking in ISWS-BUL-69/87 is relatively simple in setup, but different in approach from MODPATH. The particle tracking done in ISWS/BUL-69/87 was calculated using GWPATH, instead of MODPATH. These methods are different but can produce similar results. The grid used in ISWS/BUL-69/87 is node-based, while the grid in MODPATH is cell-based. The capture zone was created by placing 300 particles in a circle around the extraction well and reverse-tracking them for ten years.



Source: modified from ISWS/BUL-69/87

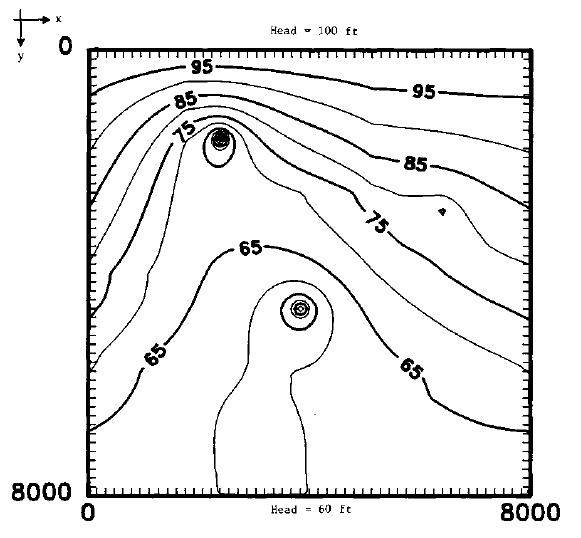
Figure 3‑8. 10-year capture zone for extraction well located at 1,170 m, 1,414 m (3,840 ft, 4,640 ft) in ISWS/BUL-69/87



Source: ISWS/BUL-69/87

Figure 3‑9. Hydraulic conductivity (ft/day) used in ISWS/BUL-69/87, and used as the basis for the hydraulic conductivity grid for MP-ATC-4 and MU-ATC-1

| **Table 3‑8. Model Properties listed in ISWS/BUL-67/87** | | | | |
| --- | --- | --- | --- | --- |
| Variable Name | Variable Value | Units | Source | |
| Model length in the x and y directions | 2,438 (8,000) | m (ft) | ISWS/BUL-67/87, Figure 19 | |
| Well 1 location (x,y) | 731, 488 (2,400, 1,600) | m (ft) | ISWS/BUL-67/87 | |
| Well 1 pumping rate | 1,090 (200) | m3/day (gpm) | ISWS/BUL-67/87 | |
| Well 2 location (x,y) | 1,951, 878 (6,400, 2,880) | m (ft) | ISWS/BUL-67/87 | |
| Well 2 pumping rate | 2,180 (400) | m3/day (gpm) | ISWS/BUL-67/87 | |
| Well 3 location (x,y) | 1,170, 1,414 (3,840, 4,640) | m (ft) | ISWS/BUL-67/87 | |
| Well 3 pumping rate | 2,725 (500) | m3/day (gpm) | ISWS/BUL-67/87 | |
| Well 4 location (x,y) | 878, 2,048 (2,880, 6,720) | m (ft) | ISWS/BUL-67/87 |
| Well 4 pumping rate | 1,635 (300) | m3/day (gpm) | ISWS/BUL-67/87 | |
| Porosity | 0.25 | N/A | ISWS/BUL-67/87 | |
| Number of particles | 300 | N/A | ISWS/BUL-67/87 | |



Source: ISWS/BUL-69/87

Figure 3‑10. Head contours used in ISWS/BUL-69/87

#### Test Case Setup

Test setup consists of six parts:

* Offset the MODFLOW grid to better match the node-based grid of ISWS/BUL-69/87.
* Digitize Figure 3‑9 in order to apply the hydraulic conductivity grid in ISWS/BUL-69/87 to the MODFLOW model grid.
* Digitize Figure 3‑8 to quantify the shape of the 10-year capture zone. This capture zone shape is used to assess the pass/fail status of this test case.
* 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 3‑8.

##### Offset the MODFLOW Grid

The particle tracking in ISWS/BUL-69/87 is done on a node-based model; MODPATH and MODFLOW are cell-based. To account for this difference, the upper left corner of the MODFLOW model was moved up and to the left by the length of half a grid cell. This put the centers of the grid cells in the MODFLOW model in the same locations as the nodes of the model in ISWS/BUL-69/87. This offset left the bottom row and right column only partially covered by grid cells, so a row was added to the bottom of the model and a column to the right to fully cover the entire modeled area.

##### Digitize the Hydraulic Conductivity Grid

The hydraulic conductivity distribution in Figure 3‑9 was digitized for use in the MODFLOW model. This process took the following steps:

1. Digitize Figure 3‑9
   1. Using a screen-capture tool, capture an image of Figure 3‑9 from ISWS/BUL-69/87 and save it as an image file.
   2. Using a script (“S00\_pngs\_2\_tiffs.py”, described more in Section 3.3.4.5) convert the image to a raster with projection information.
2. Create the model grid with the same projection information as the raster of Figure 3‑9.
   1. Use the script “S00\_create\_grid.py”, described further in Section 3.3.4.5.
   2. This creates a shapefile of the grid.
3. In a GIS program, overlay the shapefile of the grid on top of the raster of Figure 3‑9. In the attribute table, create an attribute for hydraulic conductivity, and assign the hydraulic conductivity values here.
   1. The MODFLOW grid is not perfectly aligned with the boundaries of the hydraulic conductivity zones, so professional judgment must be exercised along the boundaries of some hydraulic conductivity zones. The hydraulic conductivity assigned to the grid compared to the hydraulic conductivity zones is shown in Figure 3‑11.
   2. Save the changes to the shapefile. This shapefile will be used in model setup to assign the hydraulic conductivity in the MODFLOW files.

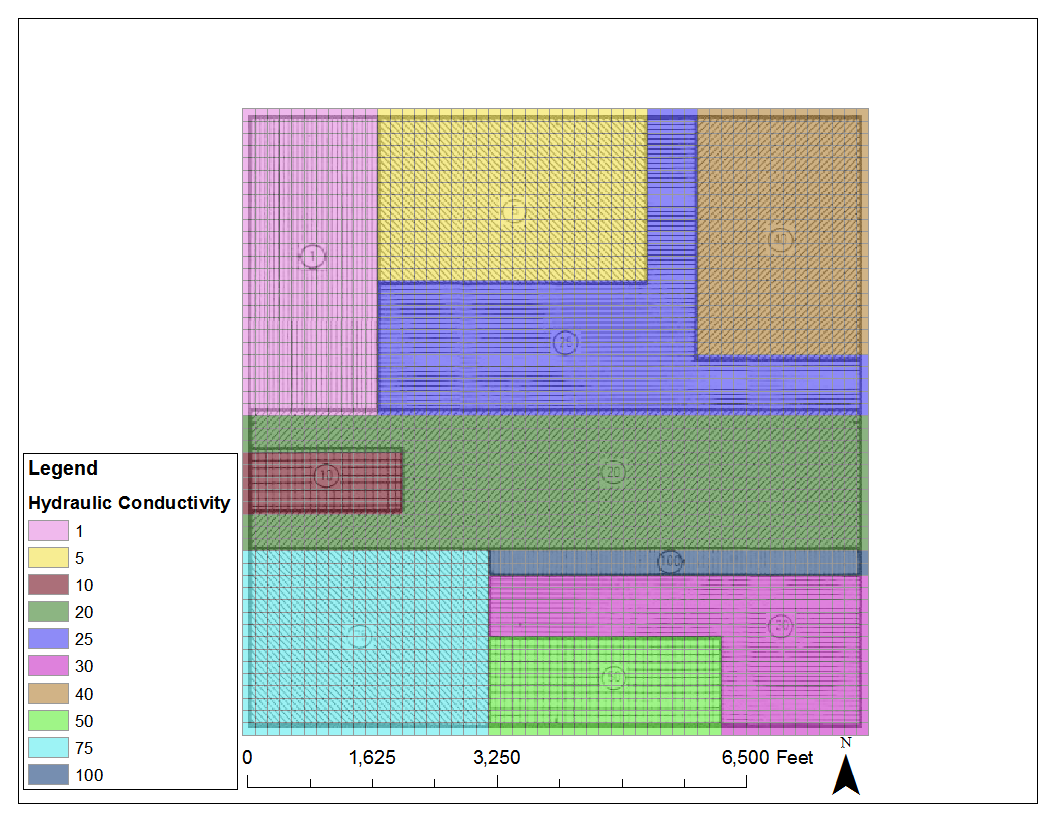


Figure 3‑11. MODFLOW hydraulic conductivity mapped against those seen in ISWS-BUL-69/87

##### Digitize the Capture Zone

Dimensions of the shape of the capture zone in Figure 3‑8 are the metrics upon which the pass/fail status of this test case rest. To get these dimensions into a format that can be compared to model outputs, Figure 3‑8 must be digitized. This process took the following steps:

1. Digitize Figure 3‑8
   1. Using a screen-capture tool, capture an image of Figure 3‑8 from ISWS/BUL-69/87 and save it as an image file.
   2. Using a script (“S00\_pngs\_2\_tiffs.py”, described more in Section 3.3.4.5) convert the image to a raster with projection information.
2. Create a shapefile defining the 10-year capture zone.
   1. Using a GIS program, create a new polygon shapefile. Open a GIS workspace with the raster of Figure 3‑8 and the new shapefile as layers. Populate the shapefile by digitizing the boundary of the 10-year capture zone from the raster of Figure 3‑8.

##### Assemble the MODFLOW Model

The MODFLOW model was assembled using the values in Pollock, 1988, when provided, and made reasonable assumptions at values needed, but not provided, by Pollock, 1988. Table 3‑9 lists the model length and number of cells, well data, and stress period data. The constant head data for the left and right boundaries, which represent a linear stepdown from 30.48 (100) to 18.29 (60) m (ft), were calculated using a script and shown in Table 3‑10. The hydraulic conductivity grid data was read from the shapefile created in 3.3.4.2.2 and applied to the proper MODFLOW file.

| Table 3‑9. Model Properties Used in MP-ATC-4 and MU-ATC-1 | | | |
| --- | --- | --- | --- |
| Variable Name | Variable Value | Units | Source |
| Model length in the x and y directions | 2,487 (8,160) | m (ft) | Modified from ISWS/BUL-69/87 |
| Number of cells in the x and y directions | 51 | N/A | Modified from ISWS/BUL-69/87 |
| Well 1 location (row, column) | 11, 16 | N/A | Assumed from ISWS/BUL-69/87 |
| Well 1 pumping rate | 1,090 (38,500) | m3/day (ft3/day) | ISWS/BUL-69/87 |
| Well 2 location (row, column) | 19, 41 | N/A | Assumed from ISWS/BUL-69/87 |
| Well 2 pumping rate | 2,180 (77,000) | m3/day (ft3/day) | ISWS/BUL-69/87 |
| Well 3 location (row, column) | 30, 25 | N/A | Assumed from ISWS/BUL-69/87 |
| Well 3 pumping rate | 2,725 (96,250) | m3/day (ft3/day) | ISWS/BUL-69/87 |
| Well 4 location (row, column) | 43, 19 | N/A | Assumed from ISWS/BUL-69/87 |
| Well 4 pumping rate | 1,635 (57,750) | m3/day (ft3/day) | ISWS/BUL-69/87 |
| Number of particles | 100 | N/A | Modified from ISWS/BUL-69/87 |
| Number of stress periods | 10 | N/A | ISWS/BUL-69/87 |
| Stress period length | 365.25 | days | ISWS/BUL-69/87 |

| Table 3‑10. Constant Head Boundary Cell Values for the East and West Boundaries in MP-ATC-4 and MU-ATC-1 | | | | | | | |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Constant Head Boundary Cells | |  | Constant Head Boundary Cells | |  | Constant Head Boundary Cells | |
| Row | Head (m[ft]) |  | Row | Head (m[ft]) |  | Row | Head (m[ft]) |
| 1 | 30.5 (100.0) |  | 18 | 26.3 (86.4) |  | 35 | 22.2 (72.8) |
| 2 | 30.2 (99.2) |  | 19 | 26.1 (85.6) |  | 36 | 21.9 (72.0) |
| 3 | 30.0 (98.4) |  | 20 | 25.8 (84.8) |  | 37 | 21.7 (71.2) |
| 4 | 29.7 (97.6) |  | 21 | 25.6 (84.0) |  | 38 | 21.5 (70.4) |
| 5 | 29.5 (96.8) |  | 22 | 25.4 (83.2) |  | 39 | 21.2 (69.6) |
| 6 | 29.3 (96.0) |  | 23 | 25.1 (82.4) |  | 40 | 21.0 (68.8) |
| 7 | 29.0 (95.2) |  | 24 | 24.9 (81.6) |  | 41 | 20.7 (68.0) |
| 8 | 28.8 (94.4) |  | 25 | 24.6 (80.8) |  | 42 | 20.5 (67.2) |
| 9 | 28.5 (93.6) |  | 26 | 24.4 (80.0) |  | 43 | 20.2 (66.4) |
| 10 | 28.3 (92.8) |  | 27 | 24.1 (79.2) |  | 44 | 20.0 (65.6) |
| 11 | 28.0 (92.0) |  | 28 | 23.9 (78.4) |  | 45 | 19.7 (64.8) |
| 12 | 27.8 (91.2) |  | 29 | 23.7 (77.6) |  | 46 | 19.5 (64.0) |
| 13 | 27.6 (90.4) |  | 30 | 23.4 (76.8) |  | 47 | 19.3 (63.2) |
| 14 | 27.3 (89.6) |  | 31 | 23.2 (76.0) |  | 48 | 19.0 (62.4) |
| 15 | 27.1 (88.8) |  | 32 | 13.8 (75.2) |  | 49 | 18.8 (61.6) |
| 16 | 26.8 (88.0) |  | 33 | 22.7 (74.4) |  | 50 | 18.5 (60.8) |
| 17 | 26.6 (87.2) |  | 34 | 22.4 (73.6) |  | 51 | 18.3 (60.0) |

##### Assemble the MODPATH Model

Setup for the MODPATH model required defining the locations of the particles, as well as the porosity. ISWS/BUL-69/87 states that the porosity is 0.25. Around Well 3, 100 particles were placed, evenly spaced, in a circle with a diameter of 15.2 m (50 ft). Their locations in the model are seen in Table 3‑11.

| Table 3‑11. Particle Starting Locations for Reverse Particle Tracking in MP-ATC-4 and MU-ATC-1 | | | | | | | | | | | | |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Particle ID | Row | Column | Local X | Local Y | Local Z |  | Particle ID | Row | Column | Local X | Local Y | Local Z |
| 1 | 30 | 25 | 0.8125 | 0.5 | 0.5 |  | 51 | 30 | 25 | 0.1875 | 0.5 | 0.5 |
| 2 | 30 | 25 | 0.811883 | 0.519622 | 0.5 |  | 52 | 30 | 25 | 0.188117 | 0.480378 | 0.5 |
| 3 | 30 | 25 | 0.810036 | 0.539167 | 0.5 |  | 53 | 30 | 25 | 0.189964 | 0.460833 | 0.5 |
| 4 | 30 | 25 | 0.806965 | 0.558557 | 0.5 |  | 54 | 30 | 25 | 0.193035 | 0.441443 | 0.5 |
| 5 | 30 | 25 | 0.802682 | 0.577716 | 0.5 |  | 55 | 30 | 25 | 0.197318 | 0.422284 | 0.5 |
| 6 | 30 | 25 | 0.797205 | 0.596568 | 0.5 |  | 56 | 30 | 25 | 0.202795 | 0.403432 | 0.5 |
| 7 | 30 | 25 | 0.790555 | 0.615039 | 0.5 |  | 57 | 30 | 25 | 0.209445 | 0.384961 | 0.5 |
| 8 | 30 | 25 | 0.782758 | 0.633056 | 0.5 |  | 58 | 30 | 25 | 0.217242 | 0.366944 | 0.5 |
| 9 | 30 | 25 | 0.773846 | 0.650548 | 0.5 |  | 59 | 30 | 25 | 0.226154 | 0.349452 | 0.5 |
| 10 | 30 | 25 | 0.763852 | 0.667446 | 0.5 |  | 60 | 30 | 25 | 0.236148 | 0.332554 | 0.5 |
| 11 | 30 | 25 | 0.752818 | 0.683683 | 0.5 |  | 61 | 30 | 25 | 0.247182 | 0.316317 | 0.5 |
| 12 | 30 | 25 | 0.740785 | 0.699195 | 0.5 |  | 62 | 30 | 25 | 0.259215 | 0.300805 | 0.5 |
| 13 | 30 | 25 | 0.727803 | 0.713921 | 0.5 |  | 63 | 30 | 25 | 0.272197 | 0.286079 | 0.5 |
| 14 | 30 | 25 | 0.713921 | 0.727803 | 0.5 |  | 64 | 30 | 25 | 0.286079 | 0.272197 | 0.5 |
| 15 | 30 | 25 | 0.699195 | 0.740785 | 0.5 |  | 65 | 30 | 25 | 0.300805 | 0.259215 | 0.5 |
| 16 | 30 | 25 | 0.683683 | 0.752818 | 0.5 |  | 66 | 30 | 25 | 0.316317 | 0.247182 | 0.5 |
| 17 | 30 | 25 | 0.667446 | 0.763852 | 0.5 |  | 67 | 30 | 25 | 0.332554 | 0.236148 | 0.5 |
| 18 | 30 | 25 | 0.650548 | 0.773846 | 0.5 |  | 68 | 30 | 25 | 0.349452 | 0.226154 | 0.5 |
| 19 | 30 | 25 | 0.633056 | 0.782758 | 0.5 |  | 69 | 30 | 25 | 0.366944 | 0.217242 | 0.5 |
| 20 | 30 | 25 | 0.615039 | 0.790555 | 0.5 |  | 70 | 30 | 25 | 0.384961 | 0.209445 | 0.5 |
| 21 | 30 | 25 | 0.596568 | 0.797205 | 0.5 |  | 71 | 30 | 25 | 0.403432 | 0.202795 | 0.5 |
| 22 | 30 | 25 | 0.577716 | 0.802682 | 0.5 |  | 72 | 30 | 25 | 0.422284 | 0.197318 | 0.5 |
| 23 | 30 | 25 | 0.558557 | 0.806965 | 0.5 |  | 73 | 30 | 25 | 0.441443 | 0.193035 | 0.5 |
| 24 | 30 | 25 | 0.539167 | 0.810036 | 0.5 |  | 74 | 30 | 25 | 0.460833 | 0.189964 | 0.5 |
| 25 | 30 | 25 | 0.519622 | 0.811883 | 0.5 |  | 75 | 30 | 25 | 0.480378 | 0.188117 | 0.5 |
| 26 | 30 | 25 | 0.5 | 0.8125 | 0.5 |  | 76 | 30 | 25 | 0.5 | 0.1875 | 0.5 |
| 27 | 30 | 25 | 0.480378 | 0.811883 | 0.5 |  | 77 | 30 | 25 | 0.519622 | 0.188117 | 0.5 |
| 28 | 30 | 25 | 0.460833 | 0.810036 | 0.5 |  | 78 | 30 | 25 | 0.539167 | 0.189964 | 0.5 |
| 29 | 30 | 25 | 0.441443 | 0.806965 | 0.5 |  | 79 | 30 | 25 | 0.558557 | 0.193035 | 0.5 |
| 30 | 30 | 25 | 0.422284 | 0.802682 | 0.5 |  | 80 | 30 | 25 | 0.577716 | 0.197318 | 0.5 |
| 31 | 30 | 25 | 0.403432 | 0.797205 | 0.5 |  | 81 | 30 | 25 | 0.596568 | 0.202795 | 0.5 |
| 32 | 30 | 25 | 0.384961 | 0.790555 | 0.5 |  | 82 | 30 | 25 | 0.615039 | 0.209445 | 0.5 |
| 33 | 30 | 25 | 0.366944 | 0.782758 | 0.5 |  | 83 | 30 | 25 | 0.633056 | 0.217242 | 0.5 |
| 34 | 30 | 25 | 0.349452 | 0.773846 | 0.5 |  | 84 | 30 | 25 | 0.650548 | 0.226154 | 0.5 |
| 35 | 30 | 25 | 0.332554 | 0.763852 | 0.5 |  | 85 | 30 | 25 | 0.667446 | 0.236148 | 0.5 |
| 36 | 30 | 25 | 0.316317 | 0.752818 | 0.5 |  | 86 | 30 | 25 | 0.683683 | 0.247182 | 0.5 |
| 37 | 30 | 25 | 0.300805 | 0.740785 | 0.5 |  | 87 | 30 | 25 | 0.699195 | 0.259215 | 0.5 |
| 38 | 30 | 25 | 0.286079 | 0.727803 | 0.5 |  | 88 | 30 | 25 | 0.713921 | 0.272197 | 0.5 |
| 39 | 30 | 25 | 0.272197 | 0.713921 | 0.5 |  | 89 | 30 | 25 | 0.727803 | 0.286079 | 0.5 |
| 40 | 30 | 25 | 0.259215 | 0.699195 | 0.5 |  | 90 | 30 | 25 | 0.740785 | 0.300805 | 0.5 |
| 41 | 30 | 25 | 0.247182 | 0.683683 | 0.5 |  | 91 | 30 | 25 | 0.752818 | 0.316317 | 0.5 |
| 42 | 30 | 25 | 0.236148 | 0.667446 | 0.5 |  | 92 | 30 | 25 | 0.763852 | 0.332554 | 0.5 |
| 43 | 30 | 25 | 0.226154 | 0.650548 | 0.5 |  | 93 | 30 | 25 | 0.773846 | 0.349452 | 0.5 |
| 44 | 30 | 25 | 0.217242 | 0.633056 | 0.5 |  | 94 | 30 | 25 | 0.782758 | 0.366944 | 0.5 |
| 45 | 30 | 25 | 0.209445 | 0.615039 | 0.5 |  | 95 | 30 | 25 | 0.790555 | 0.384961 | 0.5 |
| 46 | 30 | 25 | 0.202795 | 0.596568 | 0.5 |  | 96 | 30 | 25 | 0.797205 | 0.403432 | 0.5 |
| 47 | 30 | 25 | 0.197318 | 0.577716 | 0.5 |  | 97 | 30 | 25 | 0.802682 | 0.422284 | 0.5 |
| 48 | 30 | 25 | 0.193035 | 0.558557 | 0.5 |  | 98 | 30 | 25 | 0.806965 | 0.441443 | 0.5 |
| 49 | 30 | 25 | 0.189964 | 0.539167 | 0.5 |  | 99 | 30 | 25 | 0.810036 | 0.460833 | 0.5 |
| 50 | 30 | 25 | 0.188117 | 0.519622 | 0.5 |  | 100 | 30 | 25 | 0.811883 | 0.480378 | 0.5 |

##### 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 3.3.4.5.

#### 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, instead of MODPATH. This may have resulted in some differences in the capture zone shape, as the underlying method uses a different equation to solve for the particle locations.

#### File Structure

All files for MP-ATC-4 are contained within the “Test\_Case\_4” 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\_20\_block\_hk\_polygon.shp and related files
    - Description: This is a shapefile of the model grid with hydraulic conductivity information attached. It can be seen in Figure 3‑11, overlain on the hydraulic conductivity map from 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 3‑8. Information about the raster version of Figure 3‑8 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)
    - head\_contour.shp and related files
      * Description: This shapefile shows the contours of head in the MODFLOW model. This file can be used to compare against the head values shown in Figure 3‑10. This comparison is not part of the pass/fail criteria.
    - mp6\_10\_yrs\_poly.shp and related files
      * Description: This shapefile shows the ten-year capture zone created in this test case. This shapefile is used during post-processing to calculate the pass/fail status of this test case.
  + contour\_head.png
    - Description: This image file shows the MODFLOW head values. This file can be used to compare against the head values shown in Figure 3‑10. This comparison is not part of the pass/fail criteria.
  + pathline.png
    - Description: This image file shows the particle pathlines in MODPATH that define the capture zone for this test case.
  + tc4\_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.
* /preprocessing (This folder contains data used in model calculation or post-processing. These data are static and do not need to be re-calculated every time the model is run.)
  + /gwpath\_images (This folder contains images copied from Pollock, 1988)
    - fig\_19\_head.png
      * Description: an image file of Figure 3‑10. This was captured from a digital version of ISWS/BUL-69/87 using a screen-capture tool.
    - fig\_20\_block\_hk.png
      * Description: an image file of Figure 3‑9. This was captured from a digital version of ISWS/BUL-69/87 using a screen-capture tool.
    - fig\_21\_capture\_zone.png
      * Description: an image file of Figure 3‑8. This was captured from a digital version of ISWS/BUL-69/87 using a screen-capture tool.
  + /gwpath\_rasters (This folder contains the rasters created from the images in /gwpath\_images)
    - fig\_19\_head.tif
      * Description: The raster of “fig\_19\_head.png” created by “S00\_pngs\_2\_tiffs.py”.
    - fig\_20\_block\_hk.tif and associated aux file
      * Description: The raster of “fig\_20\_block\_hk.png” created by “S00\_pngs\_2\_tiffs.py”.
    - fig\_21\_capture\_zone.tif and associated aux file
      * Description: The raster of “fig\_21\_capture\_zone.png” created by “S00\_pngs\_2\_tiffs.py”.
    - Starting\_location.shp and related files
      * Description: A point file which defines the arbitrarily-selected location of the upper-left corner of the figures during the digitization process.
  + grid\_offset\_51.shp and related files
    - Description: This is a shapefile of the model grid with the hydraulic conductivity values assigned to every cell, as described in Section 3.3.4.2.2. This is the grid shapefile seen in Figure 3‑11. This shapefile was created by “S00\_create\_grid.py” and edited to contain hydraulic conductivity values.
  + S00\_create\_grid.py
    - Description: This python script creates the shapefile of the model grid (grid\_offset\_51.shp) and assigns it the same projection as the rasters in /gwpath\_rasters.
  + S00\_pngs\_2\_tiffs.py
    - Description: This python script digitizes an image and assigns it an arbitrary projection. This is done so the model locations depicted in the image can be defined and used as incomes for this test, or be compared to the outcomes of this test.
  + texas\_gam.prj
    - Description: projection data for the projection arbitrarily selected for use in this test case.
* /workspace (This folder is empty before the test cases are run, but will be populated with all the MODFLOW and MODPATH files used in the test case).
  + Many of the test files which will be populated here each are titled “test\_case\_4”, and end with the following file types, listed in alphabetical order: BAS, CHD, DIS, LPF, NAM, OC, PCG, WEL, CBC, GLO, LIST, HDS, MPBAS, MPNAM, MPSIM, MPEND, MPLST, MPPTH
  + starting\_locs.csv
    - Description: this is the file of starting location points. It must match Table 3‑11 for the data present in both.
  + starting\_locs.loc
    - Description: this is the file of starting location points used in MODPATH. It must match Table 3‑11 for the data present in both.
  + MPATH6.LOG
    - Description: This is a log file created by MODPATH.
* runme.bat
  + Description: A batch file which executes S01\_tc2.py. Called by the runme.bat file in the root directory.
* S01\_tc4.py
  + Description: A python script that creates the files for the MODFLOW and MODPATH models and executes the models. This script does some post-processing: it creates the output shapefiles.
* S02\_post\_process.py
  + Description: This script calculates and prints the pass/fail status of the test to “tc4\_results.csv” in /output.
* texas\_gam.prj
  + Description: projection data for the projection arbitrarily selected for use in this test case.

### MU-ATC-1: Capture Zone in a Heterogeneous Aquifer

#### Test Case Description

MU-ATC-1 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 MP-ATC-4. Refer to Section 3.3.4.1 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

MU-ATC-1 uses the MODFLOW files from MP-ATC-4. These files were copied from MP-ATC-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 MP-ATC-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

Setup for the MODPATH model required defining the locations of the particles, as well as the porosity. ISWS/BUL-69/87 states that the porosity is 0.25. Around Well 3, 100 particles were placed, evenly spaced, in a circle with a diameter of 50 ft.

##### 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 3.3.5.4.

#### 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 MU-ATC-1 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 3‑8. Information about the raster version of Figure 3‑8 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. This script prints the pass/fail statuses of the criteria, as well as the data used to calculate those statuses to “tc5\_results.csv” in /output
* 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.

# OPERATIONAL TESTING

The MODFLOW and MT3DMS software will be subjected to operational periodic testing under a graded approach. It is recognized that computational software of this type will only change in performance under three possible conditions:

1. hardware change
2. computational software change
3. operating system (environment) change

The first type of change (in hosting hardware) is already addressed through the requirement for software installation and checkout (Section 3.3) which must be repeated to qualify any new installation of the software on new hardware.

The second type of change (in the computational software itself) is already addressed by the requirement to perform all of the acceptance tests provided in this test plan, issue a revision to the software acceptance test report to document the results of this testing, and promote the new version to production use.

The third type of change represents the one condition that must be monitored by users. Here, even patches to the operating system constitute a change to the configuration of the operating system. Accordingly, users are required to re-test their installation using Test Cases MF-ITC-1 and MT-ITC-1 before use for decision-informing calculations if their operating system configuration has changed since the last installation test was checked. Performance of this operational testing is assigned to software users for single-user systems (e.g., Windows™ workstations that are subject to frequently, even weekly, operating system patches), but will be performed by the software owner or designee for multi-user operating systems (e.g., Linux™ cluster systems that require only infrequent patches with advance notice by system administrators).

# REFERENCES

CP-47631, *Model Package Report: Central Plateau Groundwater Model*

ECF-Hanford-17-0241, *Hydraulic Gradient and Velocity Calculations for RCRA Sites in 2017* [*https://pdw.hanford.gov/arpir/pdf.cfm/viewDoc?accession=0066390H*](https://pdw.hanford.gov/arpir/pdf.cfm/viewDoc?accession=0066390H)*.*

Grubb, 1993, *Analytical Model for Estimation of Steady-State Capture Zones of Pumping Wells in Confined and Unconfined Aquifers*

ISWS/BUL-69/87, *GWPATH: Interactive Ground-Water Flow Path Analysis*

Pollock, 1988, *Semianalytical Computation of Path Lines for Finite-Difference Models*

**Acronyms, Abbreviations, and Definitions**

| Acronym | Description |
| --- | --- |
| ATR | Acceptance Test Report |
| CHPRC | CH2M HILL Plateau Remediation Company |
| FRD | Functional Requirements Document |
| MKS Integrity™ | Configuration management system software |
| MODFLOW | MODular three-dimensional finite-difference ground-water FLOW model (software) |
| MT3DMS | modular three-dimensional, multi-species transport model for simulation of advection, dispersion, and chemical reactions of contaminants in groundwater systems (software) |
| SMP | Software Management Plan |
| STP | Software Test Plan |
| USGS | U.S. Geological Survey |

# ATTACHMENTS

1. Template: Test Log for MP-ATC-1
2. Template: Test Log for MU-ATC-1

ATTACHMENT 1

Test Log for MODPATH Acceptance Test Case 1 (MP-ATC-1)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| MODFLOW Acceptance Test Case 1  Description: Forward Particle Tracking from an Injection Well | | | Test Case #: Mp-ATC-1 | | Date: | |
| System Attributes:  Version #:  Release #:  Environment:  Server: | | | Test Performed by: | | | |
| Test Step # | Requirement # | Test Instruction | | Expected Result | | Actual Result |
| 1 | Obtain files for test problem from software owner | Copy files to appropriate directory | | All test cases are stored in the appropriate place on the user’s computer, and are ready for use | |  |
| 2 | Install Anaconda | Navigate to https://www.anaconda.com/download and download Python 3.6.  Run the install package and accept all the defaults in the install window until the window titled “Advanced Installation Options” is reached. In this window, activate “Add Anaconda to my PATH environment variable” by clicking the box next to it. | | Anaconda is installed and functional. | |  |
| 3 | Open Anaconda | In the windows search bar, enter “anaconda” and select “Anaconda Prompt” | | An Anaconda prompt window will appear | |  |
| 4 | Navigate to the test directory | In the Anaconda command prompt, type the following without quotation marks or brackets, “pushd [location of folder with test cases]” and hit enter | | The prompt will be in the root directory of the test cases. | |  |
| 5 | Setup the environment | In the Anaconda command prompt, type the following without quotation marks, “install\_env.bat” then hit Enter. Please note this will take 15-20 minutes. | | The Anaconda environment is downloaded. | |  |
| 6 | Activate the environment | In the Anaconda command prompt, type the following without quotation marks, “conda activate modpath\_qa”. The name before the drive location should now read “modpath\_qa”  Confirm that the environment is correct by typing “conda list” without the quotation marks, hitting enter, and ensuring that the versions of the packages match those listed in “Readme.md” in the root directory of the folder containing the test problems. | | The Anaconda environment is activated, and the correct packages are being used. | |  |
| 7 | Run the test case | Execute the batch file by typing “runme.bat” without quotes into the Anaconda prompt and hitting Enter. | | The test cases execute without error  The /workspace folder is populated with modflow and modpath files  The /outputs folder is populated | |  |
| 8 | Examine the graphic results to ensure the test criterion are met | Open “Test\_Case\_1/output/figures, and examine the three graphic files there, “2500\_days.png”, “5000\_days.png”, and “7500\_days.png”. Ensure the particles radiate outwards in straight lines. Paste the results in the “Actual Result” box. | | MODPATH acceptance test criterion are met | |  |
| 9 | Examine the percent difference results to ensure the particle tests passed. | Open “All\_tc\_results.xlsx” and ensure that in tab Test\_Case\_1 all the values in the Pass/Fail column (column E) read “pass”. Paste the results in the “Actual Result” box. | | MODPATH acceptance test criterion are met | |  |

ATTACHMENT 2

Test Log for MODPATH Acceptance Test Case 2 (MP-ATC-2)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| MODPATH Acceptance Test Case 1  Description: Theis Transient Drawdown Problem | | | Test Case #: MF-ATC-1 | | Date: | |
| System Attributes:  Version #:  Release #:  Environment:  Server: | | | Test Performed by: | | | |
| Test Step # | Requirement # | Test Instruction | | Expected Result | | Actual Result |
| 1 - 7 | If only this test case is being run, repeat steps 1 – 7 from MP-ATC-1 | Follow steps 1 – 7 from MP-ATC-1 | | MODFLOW and MODPATH have been executed and results are ready to be examined. | |  |
| 8 | Examine the graphic results to ensure the test criterion are met | Open “Test\_Case\_2/output, and examine the graphic file there, “Compared\_pathlines.png”. Ensure digitized pathlines resemble the Modpath 6 pathlines. Paste the results in the “Actual Result” box. | | MODPATH acceptance test criterion are met | |  |
| 9 | Examine the percent difference results to ensure the particle tests passed. | Open “All\_tc\_results.xlsx” and ensure that in tab Test\_Case\_2 all the values in the Pass/Fail columns (columns J and K) read “pass”. Paste the results in the “Actual Result” box. | | MODPATH acceptance test criterion are met | |  |

ATTACHMENT 3

Test Log for MODPATH Acceptance Test Case 3 (MP-ATC-3)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| MODPATH Acceptance Test Case 1  Description: Theis Transient Drawdown Problem | | | Test Case #: MP-ATC-3 | | Date: | |
| System Attributes:  Version #:  Release #:  Environment:  Server: | | | Test Performed by: | | | |
| Test Step # | Requirement # | Test Instruction | | Expected Result | | Actual Result |
| 1 - 7 | If only this test case is being run, repeat steps 1 – 7 from MP-ATC-1 | Follow steps 1 – 7 from MP-ATC-1 | | MODFLOW and MODPATH have been executed and results are ready to be examined. | |  |
| 8 | Examine the percent difference results to ensure the particle tests passed. | Open “All\_tc\_results.xlsx” and ensure that in tab Test\_Case\_3 all the values in the Pass/Fail columns (columns D, H, and K) read “pass”. Paste the results in the “Actual Result” box. | | MODPATH acceptance test criterion are met | |  |

ATTACHMENT 4

Test Log for MODPATH Acceptance Test Case 4 (MP-ATC-4)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| MODPATH Acceptance Test Case 1  Description: Theis Transient Drawdown Problem | | | Test Case #: MP-ATC-4 | | Date: | |
| System Attributes:  Version #:  Release #:  Environment:  Server: | | | Test Performed by: | | | |
| Test Step # | Requirement # | Test Instruction | | Expected Result | | Actual Result |
| 1 - 7 | If only this test case is being run, repeat steps 1 – 7 from MP-ATC-1 | Follow steps 1 – 7 from MP-ATC-1 | | MODFLOW and MODPATH have been executed and results are ready to be examined. | |  |
| 8 | Examine the percent difference results to ensure the particle tests passed. | Open “All\_tc\_results.xlsx” and ensure that in tab Test\_Case\_4 all the values in the Pass/Fail row (row 5) read “pass”. Paste the results in the “Actual Result” box. | | MODPATH acceptance test criterion are met | |  |

ATTACHMENT 5

Test Log for modPATH-3DU Acceptance Test Case 1 (MU-ATC-1)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| MODPATH Acceptance Test Case 1  Description: Theis Transient Drawdown Problem | | | Test Case #: MF-ATC-1 | | Date: | |
| System Attributes:  Version #:  Release #:  Environment:  Server: | | | Test Performed by: | | | |
| Test Step # | Requirement # | Test Instruction | | Expected Result | | Actual Result |
| 1 - 7 | If only this test case is being run, repeat steps 1 – 7 from MP-ATC-1 | Follow steps 1 – 7 from MP-ATC-1 | | MODFLOW and MODPATH have been executed and results are ready to be examined. | |  |
| 8 | Examine the percent difference results to ensure the particle tests passed. | Open “All\_tc\_results.xlsx” and ensure that in tab Test\_Case\_5 all the values in the Pass/Fail row (row 5) read “pass”. Paste the results in the “Actual Result” box. | | MODPATH acceptance test criterion are met | |  |

1. MKS is a trademark of MKS, Inc. [↑](#footnote-ref-1)