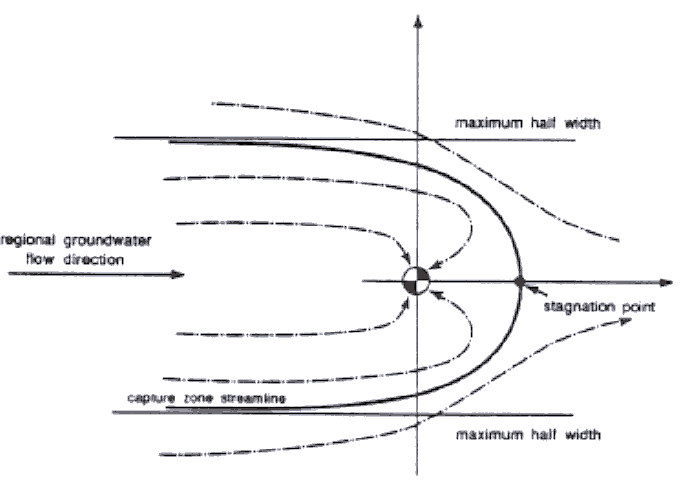
### Test Case 3: Capture Zone in an Unconfined Aquifer

**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 and estimate inputs when necessary.
* 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 number]. 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 Test Case 3 | | |
| --- | --- | --- |
| Variable name | Variable Value | Units |
| Extraction rate (Q) | 100 (19,455) | gal/min (ft3/day) |
| Hydraulic conductivity (K) | 1000 | ft/day |
| h1 head (h1) | 200 | ft |
| h2 head (h2) | 199.048 | ft |
| Distance between h1 and h2 (L) | 80,000 | 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 200-foot thick layer and is 80,000 feet long in the x direction, and 40,000 feet 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 Test Case 3 | | |
| --- | --- | --- |
| **Variable name** | **Variable Value** | **Units** |
| Pumping well location | row 401, column 1067 | N/A |
| Constant head (left) | 200 | ft |
| Constant head (right) | 199.048 | ft |
| Number of layers | 1 | N/A |
| Starting head | 200 | 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 x]. 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 Test Case 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 x].
  + 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 and “All\_tc\_results.xlsx” in the root directory.