

## Supporting Information

This document provides more detailed descriptions of some processes undertaken in the Methods section, to make it easier to recreate the model and the results produced. The processes include building the study's finite-difference model domain in ModelMuse, generating the input files for a single MODFLOW simulation, and generating a batch file for running all the MODFLOW simulations.

This study exclusively used software that is free and available for download at the addresses listed here:

- ModelMuse version 3.10.0.0:  
<https://water.usgs.gov/nrp/gwsoftware/ModelMuse/ModelMuse.html>
- MODFLOW-2005 version 1.12.0: <https://water.usgs.gov/ogw/modflow/mf2005.html>
- MT3DMS version 5.3: <https://hydro.geo.ua.edu/mt3d/index.htm>
- MODPATH version 6.0.01: <https://water.usgs.gov/ogw/modpath/>
- ZoneBudget version 3.01: <https://water.usgs.gov/nrp/gwsoftware/zonebud3/zonebudget3.html>
- R version 3.4.1: <https://mirrors.sorensgard.com/cran/>

### *A.1. Starting a New Project and Adding Programs*

Open ModelMuse and choose to “Create a new MODFLOW model”. Adding or changing geo reference data is not necessary. Specify an initial grid with 60 rows, 120 columns, and 1 layer. At this point all row and column widths are 4m. Set the “Model\_Top” elevation to 2m and the “Upper Aquifer” elevation to 0m. The grid origin has coordinates of X = 0, Y = 240, and Z = 0. Before altering anything else, go to Model > MODFLOW Options, and under the Options tab change length units to meters and time units to hours.

Some basic hydrologic parameters are constant throughout the domain but need to be changed from their default values. Under Data > Edit Data Sets, expand the Required > Hydrology data sets. The default values for the Active data set should be edited to “False”; Kx, Ky, and Kz should be changed to 3.5 (m/hr); and Modflow\_Initial\_Head should be changed to 1 (m).

All MT3DMS packages and some MODFLOW functions/post-processors need to be activated before they can be used in ModelMuse. Under Model > MODFLOW Packages and Programs, the following packages should be turned on:

- Boundary conditions > Specified head > CHD
- Boundary conditions > Head-dependent flux > EVT
- MT3DMS > BTN, ADV, DSP, SSM, GCG

- Post-processors > MODPATH, ZoneBudget

In the BTN window, make sure “MT3D Version” is set to “MT3DMS” and make one mobile chemical species with no initial concentration file. In the ADV window, the “Advection solution scheme” should be set to “Standard finite-difference method (0)”. The finite-difference solver algorithm also needs to be changed to Geometric Multigrid (Solvers > GMG), to produce acceptably low (<0.1%) discrepancies in the domain-wide water budget throughout simulations. In MODPATH > Simulation file options, “Modpath version” should be set to “6”, “ZoneArrayOption” should be checked, and “StopZone” should be set to “2”. In MODPATH > Version 6 options, “WeakSourceOption” should be set to “Stop (2)”. For ZoneBudget options, make sure “Export CSV file” and “Export CSV2 file” are both checked.

Before any objects are created, the number and type of time steps used in MODFLOW and MT3DMS should be specified. Under Model > MODFLOW Time, edit the entries of the two tabs to look like Figure S1.

MODFLOW Time

MODFLOW | MT3DMS

	Length	Max first time step length	Multiplier	Steady State/Transient
	0	0	0	

Stress period	Starting time	Ending time	Length	Max first time step length	Multiplier	Steady State/Transient	Drawdown reference	Number of steps (calculated)
1	-1	0	1	1	1	Steady state	<input checked="" type="checkbox"/>	1
2	0	720	720	1	1	Transient	<input type="checkbox"/>	720

2 Number of stress periods hours (3) Time unit (ITMUNI) Delete Insert

Convert time units ? Help OK Cancel

	Starting time	Ending time	Initial step size (DT0)	Maximum transport steps per flow step (MXSTRN)	Time step multiplier (TSMULT)	Maximum step size (TSMAX)	Steady state transport (SSFlag)
1	-1	0	0	10	1	0	<input type="checkbox"/>
2	0	1	0	200	1	0	<input checked="" type="checkbox"/>
3	1	720	0	7200	1	0	<input type="checkbox"/>

3 Number of MT3DMS periods

Convert time units Help OK Cancel

**Figure S1.** Time settings used in this model for MODFLOW (top) and MT3DMS (bottom).

#### A.2. Creating Objects

Line objects are created to hold data for the constant head (CHD) boundary conditions, the MT3DMS conservative solute, and the ZoneBudget zone representing the stream. With the “Create polyline object” tool selected, create a line with 2,400 vertices; the initial locations of the vertices do not matter. In the Object Properties window that appears after creating the line, change the object name to “CHD\_stream”. In the Vertices tab of the same window, edit the x-y coordinates of the vertices so they form a sinusoidal line with the following formula:

$$y = 15\sin((x-10)*2\pi/40)+40 \quad (S1)$$

Starting at 0.1 m, the x-values should increase in 0.2 m increments. Line objects should be created in the far left and right columns of the grid, with two vertices each; name the left line “CHD\_left” and the right line “CHD\_right”. The y-coordinates of these lines’ vertices should be changed to 28.2 and 234. Create a similar line object with two vertices in the top row of the grid, named “CHD\_top”, with x-coordinates changed to 2 and 478. For the MT3DMS solute, create a line object with 100 vertices named “MT3DMS”, then edit the x-y coordinates of those vertices to follow the sinusoidal formula mentioned above. Starting at 220.1 m, the x-values should increase in 0.2 m increments. For the ZoneBudget stream zone, create a line object named “ZB\_1” with 400 vertices. Edit the vertices so they follow the same sinusoidal formula in equation S1, starting at x = 200.1 and increasing in 0.2 m increments. In the Object Properties for ZB\_1, go to Data Sets > Required > ZoneBudget and check “Zones”. Edit the formula for the “Zones” data set to read “1”. The z-coordinates of each of these

objects (on the first tab in the Object Properties window) should be edited so they fully penetrate the single layer of the domain.

Polygon objects are needed to hold data for the evapotranspiration (EVT) boundary condition, the ZoneBudget zone representing the area of interest, the “StopZone” area for MODPATH particles, and to designate some domain cells as active (an earlier step made all cells inactive by default). The polygons all require odd numbers of vertices because the first and last vertices of all polygons must have the same coordinates for it to be considered a closed shape. In the Object Properties window of all polygons, make sure the object sets values of enclosed and intersected cells, with a minimum cell fraction of 0 unless noted otherwise.

Three of the polygon objects needed for this model have boundaries based on the sinusoidal formula from Equation S1 but set back from the stream at various distances. With the “Create polygon object” tool selected, create a polygon with 1,421 vertices and rename it “EVT”. The final x-y coordinates for the EVT polygon vertices are based on the sinusoidal formula from the previous paragraph, factoring in two setback distances from the stream: 0.4 m for the closer side of the polygon, and 30 m for the farther side. The final location of each point can be expressed as the sum of the original point’s coordinates and x and y vectors, calculated separately with:

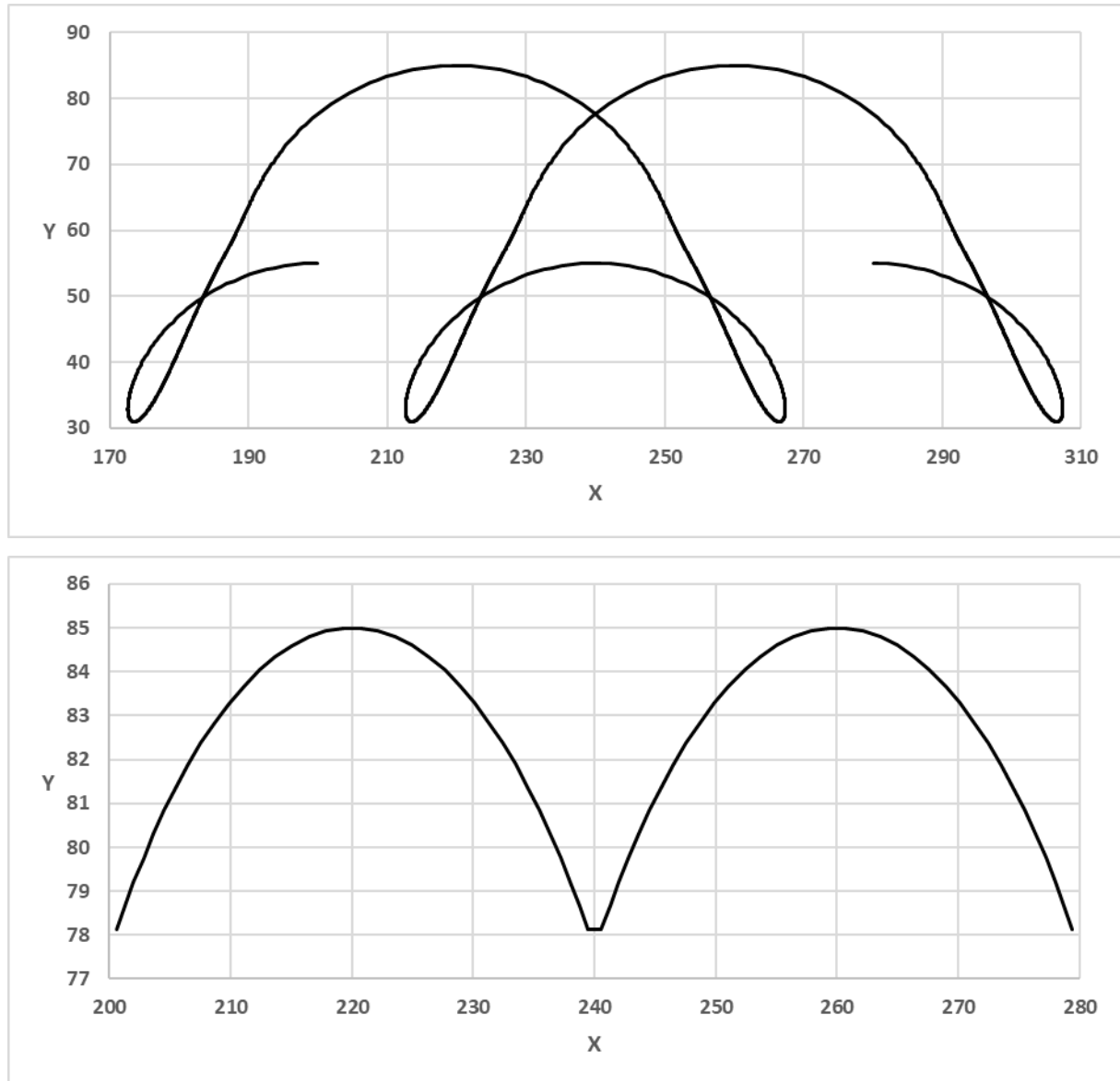
$$m_n(x) = 1/-(15\cos((x-10)*2\pi/40)) \quad (S2)$$

$$\Delta x = \Delta y/m_n \quad (S3)$$

$$\Delta y = \sqrt{(d^2x^2)/(1+x^2)} \quad (S4)$$

where  $m_n$  is the slope of the line normal to the original sine wave at a given x value,  $\Delta x$  is the x vector,  $\Delta y$  is the y vector, and d is the setback distance. Calculating these new vertex coordinates for both setback distances, based on the coordinates for the “CHD\_stream” line object for the interval  $x = [120.1, 359.9]$ , will yield more than 1,421 vertices. After removing vertices with x coordinates less than 120 or greater than 360, as well as the vertices that cause the polygon to overlap itself (Figure S2), it should finally have 1,421 vertices. In the Object Properties window, set a minimum cell fraction of 0.75. On the MODFLOW Features tab, make sure the EVT box is checked. For the ZoneBudget zone covering the area of interest, create a polygon object with 473 vertices, called ZB\_2. The vertices have coordinates identical to those used for the EVT object for the interval  $x = [200, 280]$ . Like ZB\_1, this object needs the “Zones” data set turned on, this time with a data set formula of “2”. The polygon representing the “StopZone” area for MODPATH encompasses all cells in the model except for those encompassed by ZB\_2. This was accomplished with a 483-vertex polygon named “MP\_stop”, with setback distances of 0 and 30.4 for the interval  $x = [199.7, 280.3]$ , and then additional vertices to encompass the rest of the model. In the Object Properties window, check the Data Set box for

Required > MODPATH > Modpath\_Zone, then edit the formula to "2". Finally, the object denoting active cells is a polygon named "Active" with 2,405 vertices. This polygon encompasses all the cells bounded/intersected by the 4 CHD line objects, so it uses identical vertex coordinates. Turn on the Required > Hydrology > Active data set, then edit the formula to "True".



**Figure S2.** Section of the outer boundary of the EVT polygon, before (top) and after (bottom) removing overlapping vertices.

### A.3. Adding Data to Objects

The objects representing boundary conditions need additional data to function properly for the duration of a model run. The line objects using the CHD package need to be given their constant head values. With the "Edit vertex values" tool, select the furthest-upstream vertex of CHD\_stream. Edit the key to "CHD\_stream" and the value to 1.35. Do the same to the furthest-downstream vertex, with the same key and a value of 0.75. In the Object Properties window for CHD\_stream, go to MODFLOW

Features and select the CHD package (the name, not the check box). Starting time should be set to -1 and ending time to 720. For starting head, click the gray “F()” button to edit the formula. Go to Functions > Object > InterpolatedVertexValue and double-click to add it to the formula. Edit the formula so it reads in full: InterpolatedVertexValue(“CHD\_stream”). Copy and paste this formula into the ending head box. This process should be repeated for the other three CHD objects, with unique keys for each object. This initial model domain will represent neutral regional groundwater flow, so vertices in the furthest-upstream column (column 1) should all be given values of 1.35 and vertices in the furthest-downstream column (column 306) should be given values of 0.75.

The EVT polygon object needs a full schedule of ET withdrawal rates that change between time steps. This ET schedule can be described with an equation adapted from *Gomez-Velez et al.* [29]:

$$ET(t) = \begin{cases} ET_{max} \frac{[1-\cos(wt)]}{[1-\cos(wt_p)]} & \text{if } t \in [7,18] \\ 0 & \text{otherwise} \end{cases} \quad (S5)$$

where  $t$  is the hour of the current daily cycle (e.g., active ET begins in the 7<sup>th</sup> hour and ends after the 18<sup>th</sup> hour of every day),  $ET_{max}$  is the maximum daily withdrawal rate (80 mm/day for this model setup),  $w = 2\pi/t_d$  is the event frequency,  $t_p$  is the time difference between the start of active ET and  $ET_{max}$ , and  $t_d$  is the full duration of active ET. To make the daily ET schedule symmetrical across a line between two time steps,  $t_p$  is set to 6 hr and  $t_d$  is set to 13 hr. In the MODFLOW features tab of EVT’s Object Properties window, select the EVT package and increase “Number of times” to 721. The first time step (from -1 to 0) should have an ET rate of 0, and all the subsequent time steps should have ET rates determined by Equation S5. All time steps have ET surfaces of 2 m and ET depths of 2 m.

#### A.4. Generating MODFLOW Simulation Files and a Batch File

The data contained in the ModelMuse project file must be converted to the text input files used by MODFLOW, MT3DMS, MODPATH, and ZoneBudget. Some of the input files are static across all model simulations, but others must be altered to reflect the  $J_{y/x}$  and  $ET_{max}$  being used in each scenario. A list of all input files used can be found in Table S1.

**Table S1.** Input text files needed for this study, organized by program and whether they remain static between simulations.

	MODFLOW	MT3DMS	MODPATH	ZONEBUDGET
STATIC FILES	• model.bas	• model.adv	• model.mpbas	• model.zb_response
	• model.dis	• model.btn	• model.mpn	• model.zb_zones
	• model.gmg	• model.dsp		

	<ul style="list-style-type: none"> <li>• model.lmt</li> <li>• model.lpf</li> <li>• model.nam</li> <li>• model.oc</li> </ul>	<ul style="list-style-type: none"> <li>• model.gcg</li> <li>• model.mt_nam</li> <li>• model.ssm</li> </ul>
<b>NON- STATIC FILES</b>	<ul style="list-style-type: none"> <li>• model.chd</li> <li>• model.evt</li> </ul>	

In ModelMuse, go to File > Export > MODFLOW-2005 Input Files. Copy all the static files to a new folder called “static\_files”. Copy the CHD file to a folder called “J0”, named for the neutral scenario being explored; copy the EVT file to a folder called “ET80”, named for the  $ET_{max} = 80$  mm/day scenario being explored. This step of copying non-static files to new folders needs to be repeated for all 10 scenarios of  $J_{y/x}$  and ET, which means new versions of those files need to be created. The new CHD and EVT files can come from either editing the boundary condition objects in ModelMuse and re-exporting, or manually editing the existing files.

All the files in Table S1 should now be combined in new folders, with one folder for each of the 25 simulations. The names of these folders should indicate which  $J_{y/x}$  and ET scenarios are being represented in each simulation. In this study a script written in R (“PreProcessing.R”) generated the simulation folders; filled each folder with the appropriate versions of each needed file, based on the name of the folder; and wrote a batch file to call on MODFLOW, MT3DMS, and ZoneBudget for each simulation in turn. Running the batch file will generate the text file results needed for post-processing. MODPATH is not called in the batch file because its particle tracking took longer than the time steps needed for the other programs, and therefore was simulated separately as described in Section 2.2.