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User Instructions for Tracking Particles Outside of the Grid

An option for tracking particles outside of the grid has been added to MODPATH. When activated, this option creates a file of particle locations at specified times. Particle location is computed even after a particle exits the active grid system. Particle movement outside the active grid is computed using a constant velocity that is the velocity at the exit face. After the exit, the particle location (X,Y,Z) at a time T is

$$X = XEXIT + VXE * (T-TEXIT)$$
$$Y = YEXIT+ VYE * (T-TEXIT)$$
$$Z = ZEXIT+ VZE * (T-TEXIT)$$

where

XEXITis the x coordinate at the exit face
YEXIT is the y coordinate at the exit face
ZEXIT is the z coordinate at the exit face
VXE is the X-direction velocity at the exit face
VYE is the Y-direction velocity at the exit face
VZE is the Z-direction velocity at the exit face
TEXIT is the time of exit

To use this capability, specify a file for the output in the MODPATH Name File using file type ADVOBS, and use the MODPATH Time Series option. Enter the MODPATH interactive data as usual for the Time Series option.

The ADVOBS file will contain the location of each particle at each of the "time points" specified for the TIME SERIES option. Each line in the file specifies the location of one particle at one time:

Particle number
Discharge code – 1 is not discharged, 0 is discharged
X location
Y location
Z location
Simulation time
X direction velocity upon exit (0.0 if particle has not exited)
Y direction velocity upon exit (0.0 if particle has not exited)
Z direction velocity upon exit (0.0 if particle has not exited)

While a particle is within the active grid, the (X,Y,Z) location data are the same as the location data in the Time Series file. After a particle exits, the new projected location data are written. The ENDPOINT and TIMESERS files are the same as when the TIME SERIES option is used without the ADVOBS option.

The ADVOBS file will include locations for all particles at all the specified "time points" in the time series. If the times of interest differ for different particles, then the ADVOBS file will have more data than required. For example, consider a problem in which there are measurements of two travel times, designated observations A and B. Each observation is at a different time and represents a different travel path, so MODPATH represents these using two particles, which are designated 1 and 2 in MODPATH. Observation A is at time 20 (in MODFLOW time units), and

Observation B is at time 50. Thus, there would be two times specified for the MODPATH Time Series, 20 and 50. There will be 4 lines in the ADVOBS file: the locations for particles 1 and 2 at time 20 followed by the locations for particles 1 and 2 at time 50. Observation A would be represented by the line specifying the location of particle 1 at time 20, and Observation B would be represented by particle 2 at time 50.

Example

An example problem has been made to illustrate the tracking of particles outside of the grid. Run S3 in the MODPATH documentation (USGS Open-File Report 94-464) is the basis for this problem. Run S3 tracks 20 particles along a row; some particles discharge to a well and some to a river. For this example of tracking outside the grid, only two of the particles are used. The first particle leaves the grid after 13253.3 days when it enters the cell containing the well, which is a distributed sink. This particle enters the well cell from the left. The second particle leaves the grid after 7573.73 days when it enters the river. Seepage to the river occurs out the top of the river cell as indicated by an IFACE code of 6 in the river input file for MODFLOW.

A 15000-day time series run is made using three 5000-day MODPATH time steps. Thus, the first particle discharges to the well during the third time step, and the second particle discharges to the river during the second time step. The standard MODPATH Time Series file shows only the locations of the particles prior to discharging, but the ADVOBS file will show the locations before and after they discharge.

The additional input files for this example are:

demo-s3adv.mpn – MODPATH name file, which includes a line for the ADVOBS file
demo-s3adv.loc – Starting locations file containing two particles
path-s3adv.rsp – MODPATH response file for running the ADVOBS example

The output files for this example are:

endpoint-adv.s3 – Endpoint output file
timesers-adv.s3 – Time series output file
adv.s3 – ADVOBS output file

File endpoint-adv.s3 shows particle 1 leaving the system at time 13253.3 from a location of (4010.0, 4030.0, 95.56). File adv.s3 shows the velocity of this particle upon exit as (32.926, 0.0011988, -1.0326) ft/d. Thus, at time 15000, the particle will have moved at the exit velocity for an additional 1746.7 days. This results in a movement of (57512, 2, -1804) ft, which results in a final location of (61522, 4032, -1708) ft.

Similarly, file endpoint-adv.s3 shows particle 2 leaving the system at time 7573.73 from a location of (7954, 4030, 283). File adv.s3 shows the velocity of this particle upon exit as (.31823, .0000022208, 0.20316) ft/d. Thus, at time 15000, the particle will have moved at the exit velocity for an additional 7426.27 days. This results in a movement of (2363, 0, 1509) ft, which results in a final location of (10317, 4030, 1792) ft.

Using MODPATH Particle Data in UCODE

Several steps are required to make UCODE use particle data computed by MODPATH. The purpose is to use measurements of contaminant movement, which consists of the location of a contaminant after moving for a specified time, to improve model calibration. The following information about how to do this assumes the user has already created files for running UCODE to find optimal parameters for a MODFLOW simulation using the more usual head and flow observations. In this situation, there will be a UCODE control file that references a command for running MODFLOW. This control file will have a "Command" statement in the MODEL_COMMAND_LINES section of the file for invoking MODFLOW. There will also be a file of simulated equivalents for observed heads and flows produced by the Observation capability of MODFLOW.

The first step for using the MODPATH travel time data is to modify the UCODE observation file to specify the measured travel locations. Each travel location for a specified time becomes 3 UCODE observations, the X, Y, and Z coordinates.

The second step for using the MODPATH travel time is to replace the MODFLOW command with a command that executes MODFLOW, MODPATH, and a new program named ADVOBS. MODPATH must be run after MODFLOW to compute the simulated location of the contaminant at the time of the observation. ADVOBS is a simple program that takes the particle location data from the MODPATH ADVOBS file and appends it to the end of the head and flow observation file created by MODFLOW. The easiest way to cause the 3 programs to be executed is to enter their names in a Windows ".BAT" file and modify the "Command" statement to cause UCODE to run this ".BAT" file.

ADVOBS finds the information it needs by reading file ADVOBS.DAT. ADVOBS.DAT contains the following three data items:

1. Name of the ADVOBS file produced by MODPATH
2. Name of the head and flow observation file created by MODFLOW
3. MODPATH particle number and observation time for each time-of-travel observation – one line for each observation

The third step is to create file ADVOBS.DAT. In the above example with observations A and B, the ADVOBS.DAT file would have two lines for item 3 – particle 1 at time 20 and particle 2 at time 50.

The fourth step is to modify the UCODE instruction file to specify that the simulated equivalents for the observed travel are at the end of the MODFLOW observation file. The ADVOBS program will have put the values computed by MODPATH into the MODFLOW observation file, but the user must modify the instruction file to tell UCODE how to read these simulated equivalents.