Evaluation of MODPATH/MODFLOW for groundwater residence time estimation

Prepared for

U.S. Environmental Protection Agency

in partial fulfillment of the requirements of

Clean Water Act Section 106

Grant No. I-98339411

Prepared by

James B. Palmer

Interstate Commission on the Potomac River Basin

51 Monroe Street, Suite PE-08

Rockville, MD 20850

September 2013

ICPRB Report No. ICP13-10

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Introduction

An evaluation was made of the feasibility of using the U.S. Geological Survey (USGS) MODPATH particle tracking model code and USGS's MODFLOW groundwater flow model code to estimate residence time for nutrient constituents in groundwater in a watershed. This evaluation used a MODPATH particle tracking model and a previously developed and calibrated MODFLOW-2000 flow model of the Upper Monocacy River. A number of configurations of MODPATH input parameters and parameter values were tested to define the number of groundwater particles and evaluate their impact on particle pathlines and travel times.

Model code

MODFLOW-2000 (Harbaugh and others 2000) is a computer program that numerically solves the three-dimensional ground-water flow equation for a porous medium by using a finite-difference method. (References to MODFLOW refer to the MODFLOW-2000 version of the USGS program unless otherwise identified.) MODFLOW can be instructed to record the simulation results in text listing files and binary cell-by-cell flow budget output files.

MODPATH version 6 is a "particle-tracking post-processing model that computes three-dimensional flow paths using output from groundwater flow simulations produced by MODFLOW, the U.S. Geological Survey (USGS) finite-difference groundwater flow model" (Pollock 2012). Cell-by-cell flow output files generated by MODFLOW provide groundwater velocity in every model cell and are used in MODPATH to compute paths for imaginary "particles" of water moving through the groundwater flow system. The starting locations for the particles can be automatically generated by MODPATH or defined in an input file. MODPATH also calculates the flow path length and time of travel of particles moving through the flow system. MODPATH can be configured to produce output files listing the starting and ending locations of all particles, the path of each particle and the total travel distance and time of each particle.

Upper Monocacy MODFLOW-2000 model

A calibrated MODFLOW-2000 groundwater model of the Upper Monocacy River basin was used as the groundwater flow model. A complete description of the model development, calibration and verification process is provided in Schultz and Palmer (2008). The modeled area includes the upstream tributaries of the Monocacy River in Pennsylvania and Maryland, namely Marsh, Rock, Alloway, Piney, and Toms creeks. The total area represented by the model is 309 square miles. MODFLOW simulates ground water flow using the finite difference method applied to a block-centered rectangular grid. The grid used in the Upper Monocacy River model consisted of 500 meter (m) spacing in the X- and Y- directions and ten layers of 50 m thickness in the Z-direction.

Water level observations from wells were used to calibrate the model, adjusting aquifer and streambed conductivities to provide the best match between simulated aquifer levels and a calibration dataset of water level observations. Observations for summer months (July, August and September) from years within the study period representing "average" summertime hydrologic conditions were used as targets in the calibration process. Model stream flow predictions were compared with observed values at the available gaging stations on the Monocacy River, Toms Creek, and Piney Creek. Stream flows were not used for model calibration because model recharge input data was derived from observed baseflow for these streams. A calibration comparing observed and simulated stream flow would only test the assumption that recharge in each of these watersheds eventually discharges exclusively to the stream in that watershed.

Model verification was performed by keeping all model input parameters constant except recharge parameters. Four verification runs were performed using net recharge estimates for typical net recharge during dry, average-dry, average-wet, and wet summers. Simulated water levels were compared to water level observations from available well data from years representing the hydrologic conditions corresponding to the recharge inputs. Verification runs for dry, average-dry, and average-wet conditions had good mean residuals ranging from -3.8 to 1.9 m. Residuals for the wet conditions verification run were less successful with mean residuals of -19.8 m.

Simulated flows from the model runs show the model simulates flows accurately for the Monocacy River at Bridgeport (within 3% of observed flow) and for Toms Creek (within 1%), but over-simulates flow (by up to 31%) for Piney Creek.

MODPATH version 6 is designed to be compatible with MODFLOW-2000 and MODFLOW-2005 groundwater flow models. The existing Upper Monocacy model was created to run with MODFLOW-2000. Changes were required to the existing flow model input files to output all head and flow budget output files in pure binary format without record delimiters to be compatible with MODPATH. This required minor output definition related modifications to the LPF, STR, NAM, and OC input files. All model flow simulation parameters and their values were unchanged. Input files required for MODPATH were created following instructions in the MODPATH User Guide (Pollock 2012).

The flow velocity of groundwater in the simulated flow system is calculated using the volume of water passing into and out of each cell in the model space, the porosity of the simulated aquifer material, and the dimensions of the model cells (see MODPATH User Guide (Pollock 2012) for a description of the particle tracking algorithm). For this evaluation of MODPATH the particles were assumed to be non-reactive and travel at the same velocity as the computed groundwater velocity. Cell dimensions are defined in the MODFLOW Discretization input file (with the .dis file extension) and the porosity for each model layer is defined in the MODPATH BASIC input file (with the .mpbas file extension). Flow volume through each model cell face is contained in the MODFLOW cell-by-cell budget output file.

For this evaluation of MODFLOW/MODPATH, first the MODFLOW simulation was run to produce the cell-by-cell budget output files. Then input files for a MODPATH simulation were created to use the MODFLOW output files and the simplest configuration for MODPATH. In this configuration MODPATH automatically generated the particles and their starting locations, tracked each in a forward direction and generated only an endpoint output file. This simulation ran with no errors and produced the expected endpoint file giving the starting and ending coordinates of each particle. Then the input files were changed to also output a pathline file giving the position, path length and travel time for each particle at each time step of the MODPATH simulation. Using the default configuration MODPATH generated particles in all active model cells resulting in the pathline output file taking more than 2.8 million lines of text. Rather than have MODPATH generate the particles and to reduce the number of particles simulated, a starting location file was created to define the starting location of each particle.

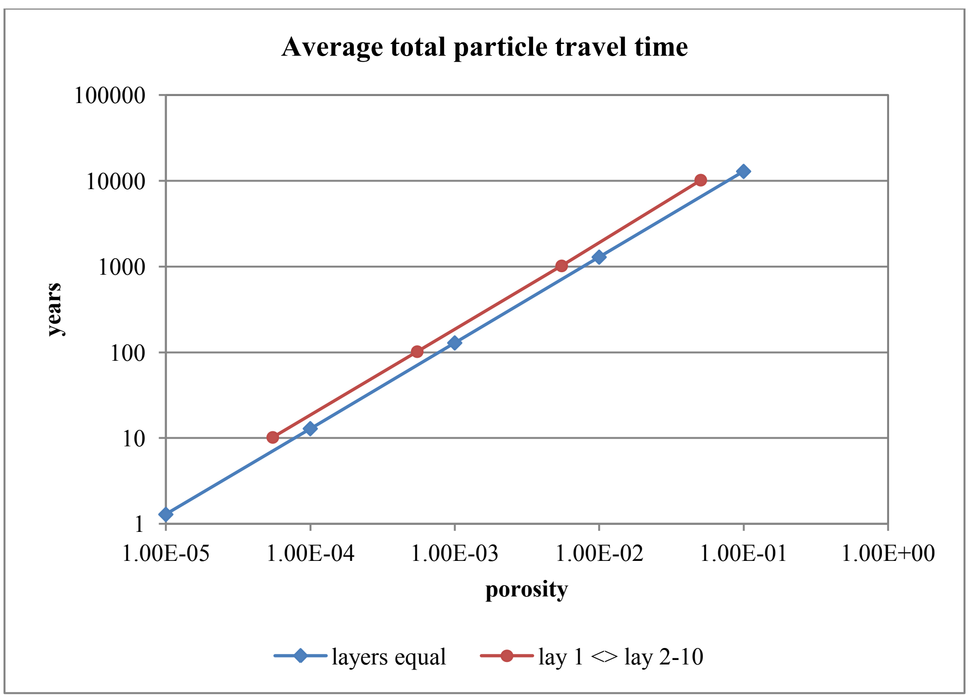
Locating a particle in each model cell produced more than 3,100 particles. Another starting location input file was made placing particles in the headwater area of the larger streams and tributaries in cells that were not dry at the end of the MODFLOW simulation. A total of 42 particles were defined for this configuration. The resulting pathline output file contained just over 1,000 lines which were imported into Excel where calculations were performed to total the path length and calculate travel time for each particle.

To evaluate the affect of porosity values on the resulting calculated travel time several simulations were performed with the 42 particle simulation described above. Starting locations of all particles were kept the same for each simulation changing only the porosity in one or more of the model layers. Initially all layers were assigned the same porosity and the values were adjusted by an order of magnitude from 1 E-01 to 1 E-05. Simulations were also run where the porosity assigned to layer 1 was an order greater than the porosity assigned to lower layers. This was to simulate the higher porosity typical in the regolith layer overlying bedrock in fractured bedrock aquifers.

Results

The MODPATH pathline output file generated by each simulation run was imported into Microsoft Excel to calculate simple statistics of total pathline length and total travel time for each simulated particle. Changing the porosity did not change the particle paths so the total pathline length remained unchanged between simulations. Travel times changed linearly with porosity between simulation runs (Figure 1).

Figure 1. Total simulated particle travel time in years versus porosity in MODPATH simulations.



Evaluation of simulation results

MODPATH as provided by USGS (http://water.usgs.gov/ogw/modpath) is accompanied by a program called MODPATH Output Examiner also produced by USGS. MODPATH output is difficult to evaluate without the assistance of post-processing tools to help visualize and examine the output. MODPATH Output Examiner is a post-processing program that allows output from MODPATH version 6 to be visualized. However, every attempt to open a MODPATH simulation using this program resulted in an error message and immediate termination of the program. The exception message indicated only that an input string was not in a correct format. Another tool would be required to provide visual representation of the calculated particle flow paths and travel times. One such tool is Groundwater Vistas by Environmental Simulations, Inc. Another tool available from USGS is ModelMuse (http://water.usgs.gov/nrp/gwsoftware/ModelMuse/ModelMuse.html), however this tool is not compatible with MODFLOW-2000 models, requiring the flow model to be modified to run in MODFLOW-2005.

Discussion

USGS's MODFLOW/MODPATH models can be used to estimate the travel time of simulated particles in groundwater. The reliability of such estimates depends on the quality of the groundwater flow simulation which depends on the quality of the input data required for a groundwater flow simulation, e.g. recharge, aquifer hydraulic conductivity, stream flow, water level observation data if used for calibration, and, of course, the quality of the conceptual model used in the development of the flow model. In addition, as shown by this evaluation the travel time estimates calculated by MODPATH are directly dependant on the porosity value assigned to each layer of the model. The existing data for the Upper Monocacy River basin model is lacking good representative porosity data for all layers in the flow model. The reliability of the particle travel times (groundwater residence time) can be improved by developing more reliable porosity data for the regolith and underlying bedrock in the modeled watersheds.

References

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