SOFTWARE RELEASE NOTICE

1. SRN Number: 315

2. Project Title: **USFIC**	Project No. 20.06002.01.131
3. SRN Title: **MODPATH, Version 3**	
4. Originator/Requestor: **James Winterle**	Date: 6/8/2004

5. Summary of Actions

- ■ Release of new software
- □ Change of access software
- □ Release of modified software:
- □ Software Retirement
  - □ Enhancements made
  - □ Corrections made

6. Validation Status

- ■ Validated
- □ Limited Validation
- □ Not Validated Explain: _____

7. Persons Authorized Access

Name	Read Only/Read-Write	Addition/Change/Delete
Executable code available to all CNWRA users. Source code is not to be modified		

8. Element Manager Approval: Gordon Wittmeyer Date: 6/8/2004

9. Remarks:
a. Existing Code: not to be modified
b. MODPATH is included as part of GMS, version 3.1, software package
c. CNWRA owns two licenses for GMS 3.1, which are accessed using a transferrable hardware lock.

SOFTWARE SUMMARY FORM

01. Summary Date:	02. Summary prepared by (Name and phone) James Winterle	03. Summary Action:
04. Software Date:	05. Short Title: MODPATH Version 3	
06. Software Title: MODPATH Version 3: A particle tracking post-processing package for MODFLOW, the U. S. Geological Survey finite-difference ground-water flow model		07. Internal Software ID:

08. Software Type: ☐ Automated Data System ■ Computer Program ☐ Subroutine/Module	09. Processing Mode: ■ Interactive ☐ Batch ☐ Combination	10. Application Area a. General: ■ Scientific/Engineering ☐ Auxiliary Analyses ☐ Total System PA ☐ Subsystem PA ☐ Other b. Specific: Groundwater Hydrology.
11. Submitting Organization and Address: CNWRA/SwRI 6220 Culebra Road San Antonio, TX 78228		12. Technical Contact(s) and Phone: James Winterle: 210-522-5249
13. Software Application: Calculates flow trajectories and velocities using MODFLOW output files.		

14. Computer Platform PC	15. Computer Operating System: Microsoft Windows 95 or later	16. Programming Language(s): N/A not to be modified	17. Number of Source Program Statements: N/A not to be modified
18. Computer Memory Requirements: Minimal (8 Mb RAM is sufficient)	19. Tape Drives: N/A	20. Disk Units: N/A	21. Graphics: No special requirements
22. Other Operational Requirements: Output can be viewed through GMS3.1 user interface or other commercial post processors			

23. Software Availability: ■ Available ☐ Limited ☐ In-House ONLY	24. Documentation Availability: ■ Available ☐ Preliminary ☐ In-House ONLY
25. Software Developer: U.S. Geological Survey Date: September, 1994	

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QA VERIFICATION REPORT
FOR
→ *ACQUIRED SOFTWARE NOT TO BE MODIFIED* ←

Software Title/Name: Modpath (Gms V. 3.1)
Version: 3.0
Demonstration workstation: Amon
Operating System: Windows NT
User: J. Winterle

NOTE: Acquired software may or may not meet all requirements and will be evaluated on a case-by-case basis.

Installation Testing [TOP-018, Section 5.6]

Has *installation testing* been conducted for each intended computer platform and operating system?
Yes: ☑ No: ☐ N/A: ☐

Computer Platforms: PC Operating Systems: Windows NT
Location of Acceptance Test Results: See enclosed TOP-18 Validation Test Plan and Validation Test.
Comments:.

Software Output [TOP-018, Section 5.5.4]

Is software designed so that individual runs are uniquely identified by date, time, name of software and version?
Yes: ☐ No: ☑ N/A: ☐

Date and Time Displayed: None
Name/Version Displayed: Modpath v 3.0
Comments:

NOTE: Output identification content and format is typically taken as is.

Medium Documentation [TOP-018, Section 5.5.6]

The physical labeling of software medium (tapes, disks, etc.) contains: Program Name, Module/Name/Title, Module Revision, File type (ASCII, OBJ, EXE), Recording Date, and Operating System(s)?
Yes: ☑ No: ☐ N/A: ☐

Comments: Copy of code in GMS (modflow96) 3.1 file.

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User Documentation [TOP-018, Section 5.5.7]

Is there a Users' Manual for the software and is it up-to-date?

Yes: ☑ No: ☐ N/A: ☐

User's Manual Version and Date: User's Guide for MODPATH / MODPATH-PLOT version 3. USGS Rpt 94-464.
Comments:

Are there basic instructions for the *installation* and *use* of the software?

Yes: ☑ No: ☐ N/A: ☐

Location of Instructions: See User's Guide
Comments: Part of GMS Package.

Configuration Control [TOP-018, Section 5.7, 5.9.3]

Is the Software Summary Form (Form TOP-4-1) completed and signed? Yes

Yes: ☑ No: ☐ N/A: ☑

Date of Approval: Acquired code.

Is the list of files attached to the Software Summary Form complete and accurate?

Yes: ☑ No: ☐ N/A: ☐

Comments: See GMS(Modflow-96) 3.1 file for record.

Is the source code available or, is the executable code available in the case of (acquired/commercial codes)?

Yes: ☑ No: ☐ N/A: ☐

Location of Source Code: _____
Comments: See GMS (Modflow 96) 3.1 file for record

Have all the ~~script/make~~ files and executable files been submitted to the Software Custodian?
Only the executable files are being submitted.

Yes: ☑ No: ☐ N/A: ☐

Location of executable files: _____
Comments: See GMS (Modflow-96) 3.1 file for record.

Software Release [TOP-018, Section 5.9]

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Upon acceptance of the software as verified above, has a Software Release Notice (SRN), Form TOP-6 been issued and does the version number of the software match the documentation?

Yes: ☑ No: ☐ N/A: ☐

SRN Number: 315

Comments:

Software Validation [TOP-018, Section 5.10]

Has a Software Validation Test Plan (SVTP) been prepared for the ***range of application*** of the software?

Yes: ☑ No: ☐ N/A: ☐

Version and Date of SVTP: June 4, 2004

Date Reviewed and Approved via QAP-002: June 4, 2004

Comments:

Has a Software Validation Test Report (SVTR) been prepared that documents the results of the validation cases, interpretation of the results, and determination if the software has been validated?

Yes: ☑ No: ☐ N/A: ☐

Version and Date of SVTR: June 4, 2004

Date Reviewed and Approved via QAP-002: June 4, 2004

Comments.:

Additional Comments:

J. R. Winterle 6-30-04 — Software Evaluator/User/Date

Randy Fedors 30 June 2004 — Software Custodian/Date

TOP-18 VALIDATION TEST PLAN AND VALIDATION TEST (COMBINED) FOR SCIENTIFIC AND ENGINEERING SOFTWARE: MODPATH, Version 3

Author: James Winterle

Code: MODPATH/MODPATH-PLOT, Version 3

Type of Code: Existing Software, Not to be Modified

Description of the Code:

The following is taken from the abstract in MODPATH/MODPATH-PLOT, Version 3, User's Guide (Pollock, 1994).

> *"MODPATH is a particle tracking post-processing package that was developed to compute three-dimensional flow paths using output from steady-state or transient ground-water-flow simulations by MODFLOW, the U. S. Geological Survey finite-difference ground-water-flow model. The particle tracking package, described in USGS Open-File Reports 89-381 and 89-622, consists of two FORTRAN computer codes: (1) MODPATH, which calculates particle paths, and (2) MODPATH-PLOT, which displays results graphically. The current report documents the most recent versions of MODPATH and MODPATH-PLOT, which were originally described in USGS Open-File Reports 89-381 and 89-622."*
>
> *"MODPATH uses a semi-analytical particle tracking scheme that allows an analytical expression of the particle's flow path to be obtained within each finite-difference grid cell. Particle paths are computed by tracking particles from one cell to the next until the particle reaches a boundary, an internal sink/source, or satisfies some other termination criterion. Data input for MODPATH and MODPATH-PLOT is a combination of data files and interactive keyboard input. Both programs are designed to work with MODFLOW. The number of new data files required by MODPATH is minimized by making use of MODFLOW data files whenever possible."*
>
> *"MODPATH and MODPATH-PLOT are written in standard FORTRAN-77. MODPATH can be compiled and run on any computer system that has a FORTRAN-77 compiler. In addition to a FORTRAN-77 compiler, MODPATH-PLOT requires a graphics subroutine library know as GKS (Graphical Kernel System). GKS is a standardized set of graphics routines that are available commercially for most computer systems."*

Acceptance Testing

In accordance with TOP-18, only installation testing is required for existing, not to be modified software. The MODPATH software was installed as part of the GMS, version 3.1 software package, which is a user interface for a variety of groundwater modeling codes. Because GMS.3.1 contains its own plotting and visualization tools, the MODPATH-PLOT code that is described in the above and in the MODPATH user's manual is not used. Hence, this validation test plan and validation test are valid only for the MODPATH code and for visualization of results through the GMS.3.1 interface. GMS 3.1 has also been separately validated under TOP-18 for

execution and visualization of the MODFLOW-96 groundwater flow modeling code. Performance of the validation exercises below, as well as previous uses of this code, indicate that this software has been successfully installed and can be easily executed through the GMS 3.1 interface.

VALIDATION TEST PLAN

The details of the validation test are provided in the following six discussion points.

1. Scope of Validation

   As discussed above MODPATH (hereafter referred to simply as MODPATH or "the code") is a particle-tracking algorithm that is intended to operate on MODFLOW output files that contain information on cell-to-cell groundwater fluxes and use that information to project groundwater flow paths and travel times from designated particle starting locations. All of these capabilities are tested by this validation test.

   Accordingly, the test plan is to start with a MODFLOW model that is already documented and look at cell-to-cell groundwater fluxes in arbitrarily selected cells. I begin with MODFLOW file from model grid 6a, run1, which corresponds to Case 2 from the Winterle (2002) report. Documentation for this MODFLOW model can be found in CNWRA Scientific Notebook 480E and input/output files are archived with the notebook on an attached CD-Rom. The steady-state solution to this model is reflected in output files that contain cell-to-cell flow budgets. From this model, I arbitrarily select a cell from within the model domain and obtain the flow budget for that cell from the MODFLOW output. I then run a MODPATH particle tracking simulation to evaluate if particle flow paths and residence times through that cell are consistent with the groundwater flow budget from the MODFLOW simulation. The following validation exercise is conducted in two parts: first is an analysis of particles distributions flowing into and out of the cell; second is an analysis of mean particle residence time in the cell.

2. References

   See Reference list at the end of this document.

3. Environment

   MODPATH/MODPATH-PLOT, Version 3, is designed to run on Microsoft Windows-based operating system. The platform used for the following validation exercises is a PC with x86 family processor; 130kb RAM, Windows NT operating system. The MODPATH code was executed through the GMS 3.1 interface.

4.0 Prerequisites

   Installation of GMS 3.1 is desirable, but MODPATH can be run in standalone mode.

   A complete set of input and output files from a properly constructed MODFLOW groundwater flow model is a necessary starting point for any MODPATH simulation.

5.0 Assumptions and Constraints

It is assumed that if MODPATH calculations are correct for a single model cell, they are also correct for multiple model cells. Hence the validation exercises are simplified greatly by evaluating particle transport calculations through a single model cell.

Additional discussion of assumptions, underlying calculations and limitations of the MODPATH code can be found in the MODPATH User's Guide (Pollack, 1994). All users are encouraged to familiarize themselves with this information.

6.0 Test Cases

Part 1 of the following Validation Test is an evaluation of particle inflow/outflow distributions calculated by MODPATH.

Part 2 of the following Validation Test is an evaluation of MODPATH particle residence time calculations.

VALIDATION TEST

Part 1: Check MODPATH Calculation of Particle Flow Distribution Within Cells

I begin with MODFLOW file from model grid 6a, run1, which corresponds to Case 2 from the Winterle (2002) report and is documented in CNWRA Scientific Notebook 480E.

I arbitrarily selected cell i=100, j=50, k=7 to test the MODPATH particle tracking. (No figure is shown, but one can imagine a single cell selected in the middle of a three-dimensional rectangular grid.) The following is the flow budget for this steady-state MODFLOW simulation (Flow units = m^3/d):

Cell to Cell Flow in:		Cell to Cell Flow out		
Upper face:	3.64373	Lower face:	-14.7983	(16.4% of inflow)
Left face:	20.2466	Right face:	-14.1465	(15.7% of inflow)
Back face:	66.1822	Front face:	-61.126	(67.9% of inflow)
Total flow in:	90.0725	Total flow out:	-90.0708	

To test that MODPATH is sending the particles the same way that MODFLOW is sending the water, I assigned a proportional number of particle to the upper, left, and back cell faces that are receiving in-flux of water. The particles are evenly distributed across each model face as follows:

Upper Face: array of 19 x 19 = 361 particles
Left Face: array of 45 x 45 = 2,025 particles
Back Face: array of 82 x 81 = 6,642 particles

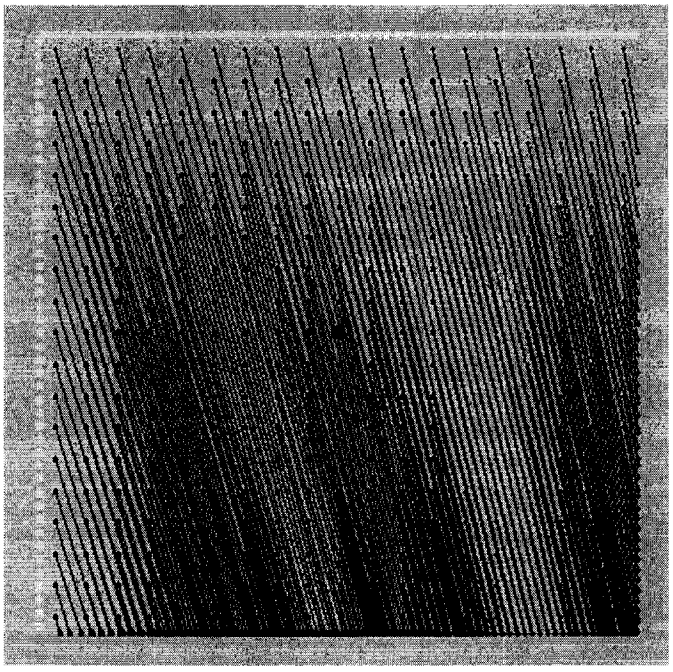
Total Particles: 9,028

These source particle assignments are approximately equivalent to shifting the decimal over two places to the right in the cell-to-cell flow in numbers. The MODPATH calculated distribution of particles flowing out of the cell faces would thus be validated if the particles flow out of the same faces and in the same proportion as the flow out in the flow budget. I set up MODPATH to terminate particle tracking at the cell faces by designating adjacent cells as the stopping points (as described in the user's manual). I then ran the code and examined the "endpoint" file, run1.ept to count the number of particles that terminate at each cell face. Cells terminating at the Lower Face are identified as having endpoints at k = 8; cells terminating at the Right Face are identified as having endpoints at i = 51; cells terminating at the Front Face are identified as having endpoints at j = 101. Results of particle end points are as follows.

Lower Face:	1468 end points	(16.2% of total particles)
Right Face:	1410 end points	(15.6% of total particles)
Front Face:	6150 end points	(68.1% of total particles)

It can thus be seen that the three-dimensional flow of particles calculated by MODPATH is proportionally consistent with the groundwater flux budget for this model cell. Differences between percent of total in-flow and percent of total particles are less than 0.2% and are mainly attributable to the fact that the numbers of particles assigned to the inflow faces are not exactly proportional to the in flow volumes. Because the particles have to be assigned in a Cartesian array on each cell face, it is not possible to assign a number of particles in exact proportion to the inflows.

As an example of the ability of GMS-3.1 to plot the MODPATH results, the following figure shows the particle paths, starting locations (light dots), and the beginning and end points for the particle tracks (dark dots) locations for particles originating from the top face of the cell. The figure is looking down on the cell in plan view with north at the top.



Part 2: Verification of MODPATH Calculation of Particle Residence Time in Model Cells

The water-filled volume of the model cell is equal to the cell volume times porosity. Cell dimensions are 300 m x 300 m x 50 m. Assigned porosity is 0.3. Water-filled volume (V), thus, comes out to be V = 1,350,000 m^3. The total inflow/outflow (Q) of 90.07 m^3/d calculated by MODFLOW would, thus, yield an average residence time (V/Q) of 14,988 days.

The MODPATH simulation discussed in Part 1 of this exercise yielded a mean particle residence time of 14,845 days. The MODPATH calculated mean residence time is within 1% of the residence time that would be expected based on an analysis of volume versus inflow/outflow. This is generally good agreement and can be considered successful validation of the MODPATH calculation of residence time in within a model cell.

Documentation of MODPATH Inputs and Outputs for Validation Exercise

Attached to this validation report is a CD-Rom with the MODPATH input and output files used in this exercise. These can be viewed to check the calculations discussed in the preceding analyses. Relevant files for the above analyses include:

> ***run1.ept***, contains endpoint data for flow paths used to evaluate distribution of particle end points
>
> ***run1.sum***, is a lengthy file that summarizes the model run; relevant information is near the end of this file, where average particle travel time is listed.

Summary and Conclusion

The preceding validation analysis demonstrates that (1) the MODPATH calculated distribution of simulated particles entering and leaving a model cell are consistent with the MODFLOW calculated flow budget to within 0.2% of the total inflow/outflow budget, and (2) MODPATH calculated mean residence time for particles flowing through this cell is consistent to within less than 1% of the residence time estimated by dividing the water-filled volume of the cell by the MODFLOW calculated inflow/outflow.

The results of these tests provide evidence that the MODPATH code has been successfully validated for the purpose of evaluating particle travel paths and travel times.

This combined Validation Test Plan and Validation Test has been developed and documented to comply with CNWRA Technical Operating Procedure TOP-018.

References

Pollack, D.W. 1994. "User's Guide for MODPATH/MODPATH-PLOT, Version 3: A particle tracking post-processing package for MODFLOW, the U. S. Geological Survey finite-difference ground-water flow model." U. S. Geological Survey Open-File Report 94-464.

Winterle, J.R. "Evaluation of Alternative Concepts for Saturated Zone Flow: Effects of Recharge and Water Table Rise on Flow Paths and Travel Times at Yucca Mountain." San Antonio, Texas: CNWRA. 2003.