Software Release Notice		
1. Software Name: Software Version: MODFLOW 2000		
2. Software Function: Finite difference groundwater flow modeling		
3. Summary of Actions: □ New Software Update to Existing Software Software Retirement		
4. Software Installation		
4a. Computer Platform(s): PC 4b. Operating System(s): Microsoft Windows NT, XP, 2000 4c. Programming Language(s): Executable only		
4d. Installation Testing: ■ Passed Performed by: <u>J. Winterle</u> Testing Performed On: <u>7/7/2005</u> Description of Testing Performed: Installed and ran groundwater model that had been previously developed using the earlier MODFLOW-96 software.		
4e. Archive Copy: ☐ Enclosed Given to IMS staff: Part of GMS 5.0 package; three GMS 5.0 licenses were purchased		
Installation Performed by: Hollen Streit	Date: 7/7/2005	
Remarks:		
5. Software Assessment		
Validation Status: ■ Full Validation □ Not Validated, Explain: Note: validation plan and validation test still in review as of 7/21/05		
Software Users: Hydrology staff. J. Winterle, Hydrology staff	Date: 7/21/05	
Remarks:		
6. Approval		
Manager: Gordon Wittmeyer Hordon Wittmeya	Date: →7/22/05	
Remarks:		
7. QA Verification		
SRN Number: 370		
Letrul	Date: 1/29/05	
Remarks:		

TOP-6-1 (6/2005)

TOP-18 VALIDATION TEST PLAN AND VALIDATION TEST REPORT (COMBINED) FOR SCIENTIFIC AND ENGINEERING SOFTWARE: MODFLOW-2000 AND GROUNDWATER MODELING SYSTEM (GMS) VERSION 5 GRAPHICAL USER INTERFACE

James Winterle

August 10, 2005

Center for Nuclear Waste Regulatory Analyses

Approved: Gordon Wittmeyer, Assistant Director Earth Sciences

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TOP-18 VALIDATION TEST PLAN AND VALIDATION TEST REPORT (COMBINED) FOR SCIENTIFIC AND ENGINEERING SOFTWARE: MODFLOW-2000 AND GROUNDWATER MODELING SYSTEM (GMS) VERSION 5 GRAPHICAL USER INTERFACE

Author: James Winterle

Date: August 10, 2005

PART 1: SOFTWARE VALIDATION TEST PLAN

Software Validated:

- MODFLOW-2000
- Groundwater Modeling System GMS, version 5.0

Type of Software: Acquired Software, Not to be Modified

Description of the Codes:

1. <u>MODFLOW-2000</u>

MODFLOW-2000 is the latest release in the series of MODFLOW codes developed by the U.S. Geological Survey. The previous release, MODFLOW-96, was validated in accordance with TOP-18 for use in regulatory reviews by CNWRA.

The following is taken from the abstract in MODFLOW 2000, User's Guide (Harbaugh, et al., 2000).

"MODFLOW is a computer program that numerically solves the three-dimensional ground-water flow equation for a porous medium by using a finite-difference method. Although MODFLOW was designed to be easily enhanced, the design was oriented toward additions to the ground-water flow equation. Frequently there is a need to solve additional equations; for example, transport equations and equations for estimating parameter values that produce the closest match between model-calculated heads and flows and measured values. This report documents a new version of MODFLOW, called MODFLOW-2000, which is designed to accommodate the solution of equations in addition to the ground-water flow equation. This report is a user's manual. It contains an overview of the old and added design concepts, documents one new package, and contains input instructions for using the model to solve the ground-water flow equation."

2. <u>GMS Version 5</u>

GMS Version 5 (GMS-5) is the latest release of the GMS groundwater modeling interface. This code is an interface used to run and visualize several different types of groundwater flow and transport models. The code is marketed by EMS-i. The somewhat self-promoting, but generally accurate, description of the GMS code found on <u>www.ems-i.com</u> is as follows:

"GMS is the most sophisticated and comprehensive groundwater modeling software available! Used by thousands of people at U.S. Government agencies, private firms,

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Author: James Winterle

Date: July 6, 2005

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and international sites in over 90 countries, it has been proven to be an effective and exciting modeling system. GMS provides tools for every phase of a groundwater simulation including site characterization, model development, calibration, post-processing, and visualization. GMS supports both finite-difference and finite-element models in 2D and 3D including MODFLOW-2000, MODPATH, MT3DMS/RT3D, SEAM3D, ART3D, UTCHEM, FEMWATER, PEST, UCODE, MODAEM and SEEP2D."

VALIDATION TEST PLAN

Validation requirements for Acquired, Not To Be Modified software are specified in Section 4 of Technical Operating Procedure TOP-018.

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

1. <u>Scope of Validation</u>—Full Validation

As discussed above the main function of MODFLOW-2000 is to numerically solve the three-dimensional ground water flow equation by using a finite difference method. This capability has been previously validated for the MODFLOW-96 code as part of the CNWRA validation of the GMS version 3.1 user interface (see master software list under GMS, MODFLOW-96). MODFLOW-96 has since been used extensively at CNWRA to develop a site-scale flow model of the Yucca Mountain area.

MODFLOW-2000 is likely to be used in analyses that support regulatory reviews. For example, the MODFLOW-96 site-scale flow model of Yucca Mountain (Winterle, 2003) will be updated to run using MODFLOW-2000. Accordingly, an appropriate validation exercise would be to ensure that MODFLOW-2000 provides similar results as a test case developed with the MODFLOW-96 version of the Yucca Mountain model. This exercise will test the MODFLOW-2000 finite difference code and also the Recharge "package," which is included with the code. Other included packages---Drain, Well, General Head Boundary, and River--were also checked as part of an installation test, but not evaluated quantitatively.

Because GMS-5 is only used as an interface to the MODFLOW model and not to perform calculations that support regulatory reviews, it is appropriate that only installation testing is necessary for validation. The use of GMS-5 to execute validation of the MODFLOW-2000 code is a suitable installation test.

2. <u>References</u>

See Reference list at the end of this document.

3. Environment

GMS-5 and the MODFLOW-2000 code included in the GMS package are designed to run on Microsoft Windows-based operating systems. The platform used for the following validation exercises is a PC with x86 family processor; 506 Mb RAM, Windows 2000 5.00 operating system. The MODFLOW-2000 code was executed through the GMS 5.1 interface.

4. <u>Prerequisites</u>

User license is required for GMS-5. Geosciences and Engineering Division presently has three licenses that were purchased from EMS-i.

5.0 Assumptions and Constraints

It is assumed that the previously validated MODFLOW-96 code is producing accurate results and, therefore, validation of MODFLOW-2000 is achieved by replication of results.

Additional discussion of assumptions, underlying calculations and limitations of the MODFLOW-2000 can be found in the User's Guide (Harbaugh, et al., 2000). All users are encouraged to familiarize themselves with this information.

6.0 Test Case and Criteria

MODFLOW-2000

The test case to be used for comparison of the MODFLOW-96 and MODFLOW-2000 models is taken from a CNWRA letter report by Winterle (2003). In that report, the chosen test case is referred to as "Run 2." This is a calibrated model of the Yucca Mountain area that includes 5 mm/yr of recharge over the potential repository area. Note: a potential point of confusion is that this model is also documented in CNWRA scientific notebook 480E, but it is referred to as "Grid S6b, Run 1" in that notebook. Since this model comparison is also documented in scientific notebook 480E, we retain the convention of referring to this model as Run 1.

The criteria for adequate replication of results between the MODFLOW-2000 and MODFLOW-96 models will be based on residual error between observed and calculated hydraulic heads at 151 observation locations within the model domain. *Replication of results will be adequate if the mean absolute error and root-mean square error for the MODFLOW-2000 test case are within 10 percent of those error values achieved for the MODFLOW-96 model.* A qualitative check on model results will also be performed by visual comparison of calculated hydraulic head contour lines plotted on the model grids for the two models; there should be no visibly distinguishable differences in contour plots from the two models.

GMS Version 5

Validation of GMS-5 will be considered successful if the software is able to display model grids, read MODFLOW input files, allow changes to MODFLOW input, execute the MODFLOW code, display observation points, calculate residual calibration error, plot hydraulic head contour lines calculated by MODFLOW, display calculated hydraulic heads for all model cells, and calculated mass fluxes at all cell faces.

PART 2: VALIDATION TEST

This validation test begins with model grid S6b and the "Run 1" set of MODFLOW input parameters and boundary conditions. The goal here is to run this version, which was initially calibrated with MODFLOW-96, with the newer MODFLOW-2000, then check to make sure the calibration and flow paths do not significantly change as a result of running the model with a different version of MODFLOW. The following bullets describe the procedure.

- Copied the S6b grid files to a new directory: D:/GMS/GMS-5
- GMS version 5.1 successfully read in the S6b grid input files with only an error message that the plot file was not compatible—this is not a problem as new plot settings were automatically generated by GMS-5 when I saved the file.
- Checked grid coordinates in the old and new GMS versions. For some reason, GMS 5.1 assigns the grid node coordinate that is a fraction of a millimeter different than the X and Y coordinates defined in the old GMS 3.1 version. For example, at i,j,k = 1,1,1 in the old version, X = 535000 m and Y = 4049000 m; however, in GMS 5.1, the same cell is assigned X = 534999.99616 and Y = 4089999.99496. Not sure why it does this, but it is not enough to make any difference.
- With the S6b grid loaded, I opened the old "run1.mfs", which is the calibrated MODFLOW-96 run for grid S6b. GMS-5 read in the file, but queried if I wanted to convert the BCF format to LPF format. LPF is an input format that can be used by MODFLOW 2000 instead of BCF. I told GMS-5 to convert and the simulation was read in with no errors.
- After reading in the run 1 simulation, I opened the MODFLOW menu for the LPF package and set the option to "use material IDs" for assigning properties to cells. Also selected "Specified Kv" as the method for assigning vertical conductivity. Checked that top 7 layers were set to "convertible" mode, which allows a switch to an unconfined solution if water level is below top of the cell.
- Checked recharge package to make sure 10 mm/yr recharge in northern area and 5 mm/yr recharge over YM area were read in correctly. All recharge cells were properly assigned.
- First attempt to run MODFLOW-2000 did not work; an error message was generated saying something about observation input was selected, but no observation was read in. I spent some time playing with the observation coverage menus in the map module. I am not sure what I did to fix the problem, but I think it was right clicking on the "Observation coverage" icon in the directory tree in the upper right pane; from that menu, I selected "Properties..." which gives a menu of options: I deselected "transport" and selected "LPF" as the flow package option. A test run of MODFLOW-2000 ran fine after this.

Based on the preceding results, installation testing of GMS, version 5 and execution of MODFLOW-2000 are considered successful.

2.2 Validation Test

After MODFLOW-2000 ran successfully, I started a new run with the starting heads in the model set to 1101 m for the top 7 layers. I then ran the model again and checked the residual observation errors. They were slightly different than the error for run 1 using GMS 3.1. I then saved the calculated heads as the new starting heads, ran the model again, and again checked the residual error. It changed slightly. A couple of more iterations of saving the new starting heads and re-running the model were done until the residual observation error no longer changed significantly. I saved this as the new calibrated model version. A comparison of the residual errors for the GMS version 3.1 (MODFLOW-96) and version 5.1 (MODFLOW-2000) are in the table below.

Comparison of residual errors for the GMS version 3.1 (MODFLOW-96) and version 5.1 (MODFLOW-2000)		
	GMS version 5.1 (Modflow-2000)	GMS version 3.1 (Modflow-96)
Mean error	0.230	0.46
Mean absolute error	9.098	8.45
Root mean square error	16.197	15.48

In general, this is a good match to the calibrated values from the old GMS 3.1 version of the model. Differences could be due to different interpolation routines used by GMS to calculate head values for observations that lie in between nodes, differences in numerical precision, or, it could just be differences in how MODFLOW-2000 converges on its final solution. It is impossible to tell without completely deconstructing both codes. In any case, the results are satisfactory.

To gain additional qualitative confidence that the model has been properly converted to the MODFLOW-2000 format, figures showing the active cells and the hydraulic head contour lines obtained from layer 6 of both models are compared on the next page. The two figures are virtually identical to the naked eye. This validation exercise provides sufficient evidence that MODFLOW-2000 works properly and the procedure described in the preceding paragraphs has successfully updated the flow model to the GMS 5.1 and MODFLOW-2000 format.

Visual Comparison of Calculated Hydraulic Head Contours for Grid S6b, Run-1, Using GMS 3.1/MODFLOW-96 (on left) and GMS 5.1/MODFLOW-2000 (On Right)



The preceding tests also demonstrate that GMS version 5 is able to display model grids, read MODFLOW input files, execute the MODFLOW code, display observation points, calculate residual calibration error, plot hydraulic head contour lines calculated by MODFLOW, and display calculated hydraulic heads for all model cells. A check was also performed to ensure that GMS-5 allows changes to MODFLOW input (via the MODFLOW menu), and that the MODFLOW-calculated mass fluxes at all cell faces can be read at any model location (via the Data menu).

2.3 Conclusions

MODFLOW-2000

Test result: Passed. MODFLOW-2000 meets the validation test criteria specified in the preceding validation test plan.

GMS Version 5

Test result: Passed. GMS-5 meets the validation test criteria specified in the preceding validation test plan.

References

Harbaugh, A.W., E.R. Banta, M.C. Hill, and M.G. McDonald. "MODFLOW-2000, The U.S. Geological Survey Modular Ground-Water Model—User Guide to Modularization Concepts and the Ground-Water Flow Process." U.S. Geological Survey Open File Report 00–92. 2000.

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.