# APPENDIX A: VERIFICATION CODES

## A1.0 MODFLOW2000

The MODFLOW ground water software has been developed by the USGS and has been continuously upgraded since the first version, MODFLOW88 was released in 1988 (McDonald and Harbaugh 2003). MODFLOW-2005 is the newest version currently available. Together, the different versions of MODFLOW have an international user base of over 1,000 users. As a ground water flow and transport simulator, the MODFLOW and related software is suited to the simulation of a wide variety of saturated zone flow and transport problems.

As part of EPA's regulatory oversight of the Waste Isolation Pilot Plant (WIPP), located in southeastern New Mexico, the U.S. Department of Energy (the Department or DOE) that operates the WIPP repository must continue to meet the certification requirements of the EPA and, in part, must demonstrate on an ongoing basis that Performance Assessment computer software is in compliance with regulations outlined in Section §194.23 – Models and Computer Codes. This section presents DOE's verification and validation of MODFLOW2000.

### A1.1 INTRODUCTION

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. MODFLOW is designed to be modular, in that different functionalities, such as wells, rivers, evapotranspiration, etc., can be added as modules to the basic ground water flow solutions. 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. The version of MODFLOW used by DOE, MODFLOW2000 (MF2K) is designed to simulate more complex boundary conditions (WIPP 2002; Donald and Harbaugh 1988; Harbaugh et al. 2000; MODFLOW 2000). The user's manual for MODFLOW 2000 (Harbaugh et al. 2000) 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. For transient and steady-state, single-phase, ground water flow problems, the MODFLOW2000 software is executed with the prescribed boundary and initial conditions. MODFLOW was not used for the CCA.

*Software Requirements* (SNL NP 19-1) requires that the following seven primary documents be developed, reviewed, and maintained for the MODFLOW software:

Software Quality Assurance (QA) Plan
Requirements Document (RD)
Verification and Validation Plan (VVP)
User's Manual (UM)
Design Document (DD)
Implementation Document (ID)
Validation Document (VD)

DOE reviewed the pre-existing documentation available for MODFLOW2000 from the USGS and found it to provide the necessary information that is usually within the RD, DD, UM, and VVP. Therefore, the only additional documents that were produced by DOE are the Software QA Plan (WIPP PA 2003c), the ID (WIPP PA 2003b), VD (WIPP PA 2003a), and the Installation and Check Out forms (WIPP PA 2003d). DOE notes that documentation for Version 1.6 will remain as the base document for any future versions of the software, with addenda for each of the documents defining the additional scope of the revised software. Configuration control is maintained through completion of Installation & Checkout (I&C) documentation for all changes made to MODFLOW2000 and system software and/or system hardware. In addition, Change Control (CC) and Software Problem Report (SPR) documents are completed, as appropriate.

The construction of newer clusters of Linux-based computers has required the testing of certain codes that have been previously qualified on older hardware.

In 2003, MODFLOW2000 Version 1.6 was qualified for use on the PC-based Linux cluster (WIPP PA 2003a). The Agency reviewed DOE's qualification and accepted the verification of MODFLOW2000 Version 1.6 on the Linux platform (EPA 2004). DOE used these EPA approved software and hardware configurations to support CRA-2004 and PABC-2004.

The Linux-based cluster was upgraded in 2006 (new processors and other hardware) and is now called the "Geo-Hydro Linux Cluster" (WIPP PA 2008). This cluster is comprised of three different hardware groups, each with a group name: (1) eleionomae, (2) pegaeae, and (3) crinaeae. The computers are connected to a job control server, "tethys.sandia.gov," which is not used for execution of codes. Because the hardware is new, but the software codes are unchanged and are not going to be recompiled, DOE only conducted regression testing to validate that the codes perform correctly on the new systems. For both CRA-2009 and PABC-2009, DOE used MODFLOW 1.6 in conjunction with the three hardware groups associated with the "Geo-Hydro Linux Cluster" mentioned above. The approach, results and Agency findings pertaining to this upgraded hardware are discussed below.

## A1.2 TEST METHODOLOGY

The DOE designed eight test cases to verify the functional requirements necessary for the verification/validation of the computer code for WIPP. The input files and corresponding output files are provided with the installation package. Listings of these files are included in Appendix A to the VD corresponding to the test number and test name. Validation testing consisted of running all test cases and checking resulting output for consistency with documented results. The test cases were run with the production executable (e.g., the executable version used for PA compliance calculations) for MF2K. The production executable was created on the target platform by the code sponsor and stored using CVS (e.g., Concurrent Versions System) version control on the target platform (CVSROOT - /h/WIPPcvs, repository - src/mf2k). The executable, source code and test problems were also stored in SCMS on the WIPP Compaq Alpha cluster (Library- MF2K, class- VER_0160).

The MF2K production executable and input and output test files were obtained from configuration management and placed in the test directories on the target platform. All of the

input files were used unmodified from the source code package, except for the **.nam* file, where the file pathnames were modified to reflect the different syntax between the Windows and Linux operating systems. The MF2K output listing files, **.lst*, created during testing were compared to the output listing files obtained from the MF2K installation package, and differences were noted and addressed. The listing file is the primary ASCII text file created by MF2K and contains an input echo, solver performance information, calculated head and a budget summary. This same procedure was used for all the tests, with the exception of Test Case 8, the algebraic multi-grid (AMG) test. The intent of Test Case 8 is to verify the Linked algebraic Multi-Grid solver (LMG) package that was not included in the MODFLOW2000 test suite. A test identical to Test Case 1, BCF2SS, was chosen, except that the solver has been switched from the Strongly Implicit Procedure (SIP) to the LMG or linked algebraic Multi-Grid solver. The results of Test Case 8 were compared to the results of Test Case 1.

After the code was verified, it was regression tested against the verification results (WIPP PA 2009a, 2009b, and 2009c). The run-control for these tests was done using the csh script RunReadScript and the Python programs ReadScript.py and Format.py. RunReadScript was used to run ReadScript.py (for processing the list of files to be checked out, checked in, executed and compared), run Fomat.py (for formatting the output of ReadScript.py into an Word file), and then check the log and Word files into the repository. The specific input script and the locations within the CVS repository where the input script and log file can be found are presented in the regression test documentation (WIPP PA 2009a, 2009b, and 2009c).

The UNIX diff (e.g., difference) command was used to compare the output to original data. The diff command does a character-by-character comparison of two ASCII files (binary files cannot be compared). Any differences are reported by listing the line number in the first file, the type of change (“a” for addition, “c” for change, “d” for deletion), and then the line numbers in the second file.

The test was considered successful if the MODFLOW2000 output listing file was the same as the documented listing file within reasonable accuracy, and accounting for date and filename changes. Reasonable accuracy was defined as numerically equal, except in the last printed digit for numbers printed with 6 or less digits, or in the digits greater than the $6^{th}$ for numbers printed with greater than 6 digits. Original output files are listed in the appendix, while the output files generated during testing were stored in CVS on the target platform and in SCMS accessible from the WIPP VMS Alpha cluster. The same criteria were used for all the test cases.

### A1.3 TEST RESULTS

The regression testing performed on the “eleionomae” cluster shows that MODFLOW2000 Version 1.6 is working in the same manner as the software performed on the original test platform.

### A1.4 THE AGENCY’S CONCLUSIONS

All test results met the acceptance criteria specified in Section 5.2 of the VD (WIPP PA 2003a). Those differences that were present were character differences, due to the addition of the build

date to the listing header, and in syntax differences between Windows and Linux pathnames, or were floating-point differences in insignificant digits. The AMG/LMG test produced very different output listings due to solver-specific output, but the head results and ground water budgets were the same as the PCG (Test Case 1, BCF2SS) results to within the acceptance criteria. Therefore, the Agency concludes that MODFLOW2000 Version 1.6 can be considered verified for use on the "eleionomae, pegaeae, and crinaeae" cluster of machines.

## A2.0 MT3D

MT3D (Modular 3D Solute Transport Model) is a comprehensive three-dimensional numerical model for simulating solute transport in complex hydrogeologic settings. MT3D has a modular design that permits simulation of transport processes independently or jointly. MT3D is capable of modeling advection in complex steady-state and transient flow fields, anisotropic dispersion, first-order decay and production reactions, and linear and nonlinear sorption. It can also handle bioplume-type reactions, monad reactions, and daughter products. This enables MT3D to do multi-species reactions and simulate or assess natural attenuation within a contaminant plume. MT3D is linked with the USGS ground water flow simulator, MODFLOW, and is designed specifically to handle advectively dominated transport problems without the need to construct refined models specifically for solute transport.

MT3D was developed by the University of Alabama's Hydrogeology Group and the verification of MT3D is provided in Zheng (2006) and Zheng and Wang (1999).

## A3.0 REFERENCES

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