MODFLOW and Related Codes

CHPRC Build 8

**ACCEPTANCE TEST REPORT**

**Signature Page**

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November 25, 2015

# OVERVIEW AND SCOPE

| Acronym: | MODFLOW | HISI ID: | 2517 | Software Grade: | C |
| --- | --- | --- | --- | --- | --- |
| Acronym: | MT3DMS | HISI ID: | 2518 | Software Grade: | C |

The objective of the testing reported in this acceptance test report (ATR) is to demonstrate applicability and suitability for use of the MODFLOW-2000, MODFLOW-2000-MST, and MT3DMS-MST software for intended uses at the Hanford Site by the CH2M-HILL Plateau Remediation Company (CHPRC).

MODFLOW-2000 is a computer code that solves the three-dimensional groundwater flow equation for a porous medium using the finite-difference numerical method. The MODFLOW code in its several versions is the most widely used code by hydrogeologists in the world to simulate the flow of groundwater through aquifers. The versions tested here include both the baseline MODFLOW-2000 distributed by the USGS as well as a variant version designated MODFLOW-2000-MST that includes code with minimum saturated thickness (MST) code modifications originally introduced by S.S. Papadopulos and Associates (SSP&A) primarily made to address the issue of dry cells becoming inactive, a limitation associated with MODFLOW and important in the Hanford hydrogeologic setting. The CHPRC Risk & Model Integration Group evaluated these code modifications previously and deemed these essential to enabling use of MODFLOW in the Hanford geologic setting. In addition, CHPRC staff received copies of and examined the validation and verification documents prepared by SSP&A for the variant version MODFLOW -2000-MST and finds these are in accordance with NQA-1-2008 requirements. Both the baseline and the variant version of MODFLOW are tested and controlled as both are needed to support CHPRC modeling needs. Moreover, both single- and double-precision versions of this software are tested as needs have been identified for both precision levels in executable code.

MT3DMS is modular three-dimensional, multi-species transport simulator to solve for advection, dispersion, and chemical reactions of contaminants in groundwater systems. It is intended for use with groundwater flow solutions calculated by the MODFLOW software. MT3DMS was obtained from SSP&A as well, with the CTS module provided for contaminant treatment system at the Hanford Site. As for the MODFLOW executable files, both single- and double-precision versions of this software are tested as needs have been identified for both precision levels in executable code.

This is the eighth revision of this ATR, reporting on acceptance testing for “CHPRC Build 8” of MODFLOW and Related Codes; the history of revisions and associated builds of this software are recounted in Table 1 below.

| Table 1. History of MODFLOW and Related Codes CHPRC Builds | | |
| --- | --- | --- |
| **ATR Revision** | **Software Build** | **Description of Changes Included in Build** |
| 0 | Build 1 | Initial acceptance testing of MODFLOW-2000-MST and MT3DMS-MST. |
| 1 | Build 2 | Inclusion of baseline MODFLOW-2000 (standard baseline MODFLOW 2000, version 1.18.01) to the software set; inclusion of Containment Treatment System (CTS) Package in MODFLOW-2000-MST and MT3DMS-MST. |
| 2 | Build 3 | Updates to MODFLOW-2000-MST and MT3DMS-MST that included further refinement of the MST features, incorporation of changes recommended by CHPRC to make the source code and file names more compatible with compilation on a Linux® platform, and inclusion of a new, faster solver (ORTHOMIN) that achieves solutions in dramatically less time. The ORTHOMIN solver, developed by HydroSOLVE, Inc., has advantages over traditional solvers available for MODFLOW. When used for flow simulations, the ORTHOMIN solver functions as an enhanced version of the preconditioned conjugate gradient method; however, coding improvements make the ORTHOMIN solver faster and computationally more efficient than the traditional PCG2 solver used in MODFLOW. |
| 3 | Build 4 | Updated MODFLOW-2000 to baseline MODFLOW-2000 Version 1.19.01 to be consistent with the basis for the new version of MODFLOW-2000-MST that adds features to this baseline version.  Updated MODFLOW-2000-MST to be compatible with baseline MODFLOW-2000 Version 1.19.01. This was completed in order to provide support to Hanford simulations for the Multi-Node Well (MNW) Version 2 (MNW2) Package. MODFLOW Version 1.18 supported MNW Version 1 (MNW1) package, which provides essentially the same capabilities as the MNW2 package: however, the MNW1 package input structure is disorganized and can lead to very complicated inputs when certain MNW capabilities are required for a simulation.  Updated MT3DMS-MST to be compatible with MT3DMS version 5.3 (v5.3). This was completed in order to provide support to Hanford simulations for the Hydrocarbon Spill Source (HSS) Package, particularly in combination with the MODFLOW flow-head boundary (FHB) package. The HSS package provides piece-wise continuous mass-loading capabilities for MT3DMS that are independent of stress periods (in a manner that is similar to the piece-wise continuous flow loading capabilities for MODFLOW provided by the FHB package). |
| 4 | Build 5 | MODFLOW-2000 is unchanged from Build 4; Version 1.19.01 has been reclassified “legacy and superseded software” by the USGS since Build 4 was qualified and no further development of this version by the USGS is expected. However, MODFLOW-2000 Version 1.19.01 is the baseline upon which MODFLOW-2000-MST is developed and so is maintained here for consistency and continued use. CHPRC modeling integration staff recently evaluated the newer, more relevant version of MODFLOW available from the USGS (MODFLOW-NWT) and determined that it presently lacks the features incorporated in MODFLOW-2000-MST necessary to adequately simulate the required features, events, and processes of groundwater flow at the Hanford Site. CHPRC will continue to monitor development of MODFLOW and reconsider this decision as capabilities evolve.  MODFLOW-2000-MST is upgraded in Build 5. The Newton-Raphson iteration method was added to MODFLOW. Because this method creates an unsymmetrical coefficient matrix, new solvers were required and added to this version as well. Other numerical techniques were also implemented.  MT3DMS-MST is upgraded in Build 5. The changes parallel and support changes in MODFLOW-2000-MST and add new capabilities. |
| 5 | Build 6 | MODFLOW-2000 is unchanged from Builds 4 and 5; Version 1.19.01 has been reclassified “legacy and superseded software” by the USGS since Build 4 was qualified and no further development of this version by the USGS is expected. However, MODFLOW-2000 Version 1.19.01 is the baseline upon which MODFLOW-2000-MST is developed and so is maintained here for consistency and continued use. CHPRC modeling integration staff recently evaluated the newer, more relevant version of MODFLOW available from the USGS (MODFLOW-NWT) and determined that it presently lacks the features incorporated in MODFLOW-2000-MST necessary to adequately simulate the required features, events, and processes of groundwater flow at the Hanford Site. CHPRC will continue to monitor development of MODFLOW and reconsider this decision as capabilities evolve.  MODFLOW-2000-MST is upgraded in Build 6. The only change is to add a dual domain *Kd* implementation.  MT3DMS-MST is unchanged from Build 5. |
| 6 | Build 7 | MODFLOW-2000 is unchanged, and remains the standard MODFLOW-2000 USGS version 1.19.01. This code has been recompiled for CHPRC Build 7 and subjected to acceptance testing.  MT3DMS is introduced in CHPRC Build 7 and acceptance tested. This provides users the option to use a qualified “stock” version of this software (that is, without the minimum saturated thickness features included in MT3DMS-MST), if appropriate  MODFLOW-2000-MST is upgraded in CHPRC Build 7. The changes include implementation of the Newton-Raphson method to provide stability in the flow solution to deal with the oscillatory behavior of the solution in the rewetting capability that has demonstrated instability in prior versions. In addition, because the Newton-Raphson method creates an unsymmetrical coefficient matrix, new solvers (PCGN, GCG, and GMR) were needed and added to this version of MODFLOW-2000-MST.These features are only available if specified by the user, in order to maintain backward compatibility.  MT3DMS-MST is upgraded in CHPRC Build 7.  Windows® and Linux® executables, in both single and double precision versions, are acceptance-tested for all four software elements. |
| 7 | Build 7 | Maintains testing performed in Revision 6, but adds MODFLOW-USG. |
| 8 | Build 8 | MODFLOW-2000-MST and MT3MDS-MST are changed to add features to support simulation of strontinum-90 incorporation mechanism. This revision tests only the new “MST” variants and retains previously tested base versions MODFLOW-2000, MT3DMS, and MODFLOW-USG. |
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The testing was conducted following CHPRC-00224, *MODFLOW and Related Codes Software Test Plan* (STP). Starting with Build 4, full acceptance testing has been performed on both the Windows®[[1]](#footnote-1) and the Linux®[[2]](#footnote-2) operating systems to confirm acceptance in both environments because both of these environments are in regular use by CHPRC to meet modeling needs. The specific hardware and operating system configurations used for acceptance testing conducted for executable files constructed in Build 7 that were unmodified in Build 8 were:

**Windows® Operating System Test Platform**

Computer Property Tag WF22668

Dell Latitude Laptop Computer

Intel® Core™ i5 CPU M540 @ 2.53 GHz

4.00 GB of RAM

Microsoft Windows 7® Enterprise Service Pack 1

**Linux® Operating System Test Platform**

Tellus Subsurface Modeling Platform - Linux® Cluster (tellusmgmt.rl.gov')

Frontend Hardware (Controller Node) is a Dell PowerEdge™[[3]](#footnote-3) M710 with Intel Xeon®[[4]](#footnote-4) X5670 dual CPU processors with 6 cores per CPU at 2.93 GHz (12 MB Cache)

96 GB of RAM

Red Hat Enterprise Linux Client release 5.8

The specific hardware and operating system configurations used for acceptance testing conducted for executable files newly constructed in Build 8 were:

**Windows® Operating System Test Platform**

Computer AUS-GALLIUM

Dell Precision T1700 Desktop Computer

Intel® Xeon® CPU E3-1270 v3 @ 3.50 GHz

8.00 GB of RAM

Microsoft Windows 10 Pro

**Linux® Operating System Test Platform**

INTERA’s Austin Linux® Cluster, with Frontend Hardware (Head Node):

1 x Intel Six Core Xeon E5-1650 3.2GHz

4 x 4GB DRx4 PC3-12800 ECC Reg. DDR3 (1600MHz)

2 x 1TB SATA 3.0Gb/s Enterprise Hard Drive 7200RPM w/ 64MB Cache with Red Hat 4.4.7-3

Testing for Build 8 was conducted by Joan Blainey, Senior Hydrologist with INTERA, Incorporated.

As Safety Software graded to level C, this ATR and test results require review by an independent technical peer reviewer (an individual with necessary technical competence who did not contribute to the creation of the STP nor participate in the conduct of the testing); this review is provided by Sunil Mehta, Senior Engineer with the CHPRC Environmental Programs and Strategic Planning organization.

The following configuration controlled items constitute the controlled software elements of CHPRC Build 8 and were subjected to acceptance testing are listed in Table 2 for Windows® executable files and in Table 3 for Linux® executable files.

For the Windows® compilations, the Lahey/Fujitsu©[[5]](#footnote-5) Fortran 95 Compiler Release 7.20.00 was used with the following compiler options to compile Fortran source code for MODFLOW-2000 and MT3DMS:

* -dbl (for double precision versions only); default double precision REAL and COMPLEX declarations, constants, functions, and intrinsics
* -ml fc specify mixed language target
* -O2 classical, memory, and interprocedural optimizations plus loop and array optimizations
* -staticlib use static Fortran libraries (linker)

Note that the executable code for Windows® was provided by the vendor (SSP&A) for MODFLOW-2000-MST and MT3MDS-MST in both single and double precision versions; these executable files were accepted for testing (rather than recompiling).

For the Linux® compilations used in the baseline MODFLOW-2000 and MT3DMS and MODFLOW-2000-MST (all constructed in Build 7 and unchanged in Build 8), the Lahey Fortran Compiler for Linux® Release 8.01b was used with the following compiler options to compile Fortran source code for MODFLOW-2000, MODFLOW-2000-MST,and MT3DMS:

* --dbl (for double precision versions only); default double precision REAL and COMPLEX declarations, constants, functions, and intrinsics
* --ml cdecl specify mixed language target
* --o3 full optimizations
* --static use static Fortran libraries (linker)
* --wide (for .f90 files only) use wide format for source
* --staticlink (for linker only) use static library linking (for portability)

For the Linux® compilations of MODFLOW-USG, the Intel® Fortran Compiler for Linux® version 13.0.1 was used with the following compiler options for MODFLOW-USG:

* -O3 full optimizations
* -autodouble (for double precision version only)
* LDFLAGS=-static -L/usr/lib/x86\_64-redhat-linux5E/lib64/ use static library linking

For the Linux® compilations of MT3DMS-MST, the Intel® Fortran Compiler for Linux® version 13.0.1 was used with the following compiler options:

* -O3 full optimizations
* --static (for linker only) use static library linking (for portability)
* -static-intel (for linker only) use static library linking for Intel-provided libraries (for portability)
* -threads Specifies that multithreaded libraries should be linked.
* -real\_size 32 (for single precision only) Defines the size of REAL and COMPLEX declarations, constants, functions, and intrinsics.
* -real size 64 (for double precision only) Defines the size of REAL and COMPLEX declarations, constants, functions, and intrinsics.

MODFLOW executable files were prepared and tested in both single- and double-precision for real variables to support work needs; certain features needed to support sub-models (telescopic mesh refinement) only work with single-precision runs while double-precision is preferred to support automated calibration using the PEST software.

No variations or deviations from the STP were necessary during the conduct of testing.

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| Table 2. MODFLOW and MT3DMS CHPRC Build 7 and8 Windows® Executable Files | | | | | |
| **Software** | **Code Source** | **Version** | **Executable File1** | **Precision** | **MD5 Signature** |
| MODFLOW-2000 | USGS 1 | Build 8 (1.19.01) | mf2k-chprc08spl.exe 2 | Single | EAF037703ADD2C62CDD9CBC47468D2F6 |
| mf2k-chprc08dpl.exe 2 | Double | 919F74196F5FB5BF0364FC373011B507 |
| MODFLOW-2000-MST | SSPA 3 | Build 8 (1.19.01) | mf2k-mst-chprc08spv.exe 4 | Single | ceb80288c616e0552e4ce5a2d4719387 |
| mf2k-mst-chprc08dpv.exe 4 | Double | 4e7f29dd5496d2cba7144adacb13daad |
| MODFLOW-USG | USGS 5 | Build 8 (1.2.00) | mfusg-chprc08spv.exe 6 | Single | 9d27bd5ece9dab4f25bcfb1aafe1d1f8 |
| mfusg-chprc08dpv.exe 6 | Double | aeaee57bb71bd299b237d4c1fc322dfb |
| MT3DMS | EPA 7 | Build 8 (5.3) | mt3d-chprc08spl.exe 2 | Single | 0920CC235862665D9400A3FC80F682DD |
| mt3d-chprc08dpl.exe 2 | Double | ECA9828530B68D2D7C34078C019D5D0C |
| MT3DMS-MST | SSPA 3 | Build 8 (5.3) | mt3d-mst-chprc08spv.exe 4 | Single | 68f89daf2e6913d2578de53cbd34fba0 |
| mt3d-mst-chprc08dpv.exe 4 | Double | 5c61432d2c898e83ddfe242c52a755ab |
| 1. Source code for Version 1.19.01 (dated March 30, 2010) downloaded from the USGS’s Ground-Water Software website <http://water.usgs.gov/nrp/gwsoftware/modflow2000/modflow2000.html> on February 25, 2015; same base version as in CHPRC Builds 4, 5 and 6. 2. Executable files compiled and linked at CHPRC using Lahey/Fujitsu© Fortran 95 Compiler Release 7.20.00. 3. Source code and Windows® executable files for Windows® downloaded from S.S. Papadopulos and Associates (SSP&A) FTP server on November 16, 2015. 4. Windows executable compiled and linked by SSP&A. 5. Source code for Version 1.2.00 (dated March 21, 2014) downloaded from the USGS’s Ground-Water Software website <http://water.usgs.gov/ogw/mfusg/> on April 29, 2015. 6. Executables were compiled and linked at INTERA using Intel® Fortran Complier for Linux® version 13.0.1. 7. Source code for Version 5.3 downloaded from maintenance site on University of Alabama’s Hydrogeology Group site <http://hydro.geo.ua.edu/mt3d/> on February 5, 2015 8. Windows executable compiled and linked by SSP&A. These files were downloaded from .S. Papadopulos and Associates (SSP&A) FTP server on November 16, 2015. The executable mf2k\_1\_18\_MST\_sngl.exe was renamed to mf2k-mst-chprc07spv.exe and mf2k\_1\_18\_MST\_sngl.exe was renamed to mf2k-mst-chprc07dpv.exe because the md5 hashes were identical. | | | | | |

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| Table 3. MODFLOW and MT3DMS CHPRC Build 8 Linux® Executable Files | | | | | |
| **Software** | **Code Source** | **Version** | **Executable File1** | **Precision** | **MD5 Signature** |
| MODFLOW-2000 | USGS 1 | Build 8 (1.19.01) | mf2k-chprc08spl.x 2 | Single | 8b0b28c5e102e63df95de542d83d013b |
| mf2k-chprc08dpl.x 2 | Double | 2fade33e27978063a9a70ff8605e4c0c |
| MODFLOW-2000-MST | SSPA 3 | Build 8 (1.19.01) | mf2k-mst-chprc08spl.x 2 | Single | be5df3a5f706cac167043fcd4b544e51 |
| mf2k-mst-chprc08dpl.x 2 | Double | 739ee01d4c2579117b4aef06c424da60 |
| MODFLOW-USG | USGS 4 | Build 8 (1.2.00) | mfusg-chprc08spl.x 5 | Single | a8a861f6d453647b100d63f064ca6af2 |
| mfusg-chprc08dpl.x 5 | Double | 682f0b1e9fcd6ac0b885f52a7ddfe821 |
| MT3DMS | EPA 6 | Build 8 (5.3) | mt3d-chprc08spl.x 2 | Single | 37ae3dcb3e56cd27e3e889a90d0ae7c1 |
| mt3d-chprc08dpl.x 2 | Double | 1be4b7d3fc81881ff0b97ff7e67bd3ff |
| MT3DMS-MST | SSPA 3 | Build 8 (5.3) | mt3d-mst-chprc08spl.x 2 | Single | 2d0a8a4c480318763b6aaaa0f880348a |
| mt3d-mst-chprc08dpl.x 2 | Double | 1e468c4409ac913843ce783aabed819c |
| 1. Source code for Version 1.19.01 (dated March 30, 2010) downloaded from the USGS’s Ground-Water Software website <http://water.usgs.gov/nrp/gwsoftware/modflow2000/modflow2000.html> on February 25, 2015; same base version as in CHPRC Builds 4, 5 and 6. 2. Executable files were compiled and linked at CHPRC using Lahey Fortran Compiler for Linux® Release 8.01b. 3. Source code and Windows® executable files for Windows® downloaded from S.S. Papadopulos and Associates (SSP&A) FTP server on November 16, 2015. 4. Source code for Version 1.2.00 (dated March 21, 2014) downloaded from the USGS’s Ground-Water Software website <http://water.usgs.gov/ogw/mfusg/> on April 29, 2015. 5. Executables were compiled and linked at INTERA using Intel® Fortran Complier for Linux® version 13.0.1. 6. Source code for Version 5.3 downloaded from maintenance site on University of Alabama’s Hydrogeology Group site <http://hydro.geo.ua.edu/mt3d/> on February 5, 2015. | | | | | |

# TEST SUMMARY

The acceptance tests specified in CHPRC-00259, *MODFLOW and Related Codes Software Test Plan*, were conducted. This document included the test plan, test design, test procedures, and test logs to use for the acceptance test cases.

## MF-ATC-1: Theis Drawdown Problem

This test is designed to calculate drawdown in an idealized uniform horizontal infinite-extent aquifer from a single fully penetrating well with constant pumping rate. An analytical solution to this problem was obtained by Theis (1935) by analogy to heat transfer and is used to validate the solution obtained in this test. Theis’ solution predicts drawdown in a confined aquifer at any distance from a well at any time since the start of pumping given the aquifer properties, transmissivity, and storage coefficient. Details of this test, the basis for the analytical solution, and expected results are presented in the STP. The test is conducted for the baseline MODFLOW-2000 version and for the MODFLOW-2000-MST variant.

### Test Results for MODFLOW-2000

The logs maintained during the conduct of this test are provided in Attachment 1 for the Windows® testing and Attachment 2 for the Linux® testing. The test was repeated in subdirectories for single and double precision executable files of this software. The expected results for drawdown with distance were calculated from the analytical solution for 5 and 10 days of pumping in either of the base validation and verification spreadsheets “mf-atc-1\_mf2k-sp.xlsx” and “mf-atc-1\_mf2k-dp.xlsx” and are presented graphically in Figure 1. Note these are the results prepared for Build 5; because the executable files for Build 6 are identical for MODFLOW-2000 retesting was not necessary.

The results were copied from the MODFLOW-2000 produced output list files named “mf-atc-1.lst” in each instance of this test for drawdown at the respective times 5 and 10 days using a text editor program and pasted into directly to cells in copies of the Microsoft Excel®[[6]](#footnote-6) spreadsheet “mf-atc-1\_mf2k-sp.xlsx” and “mf-atc-1\_mf2k-dp.xlsx” containing the analytical results. Graphically, the comparison of solutions is provided in Figure 2 for the single precision tests. For the double precision tests, the results appear in Figure 3.

The acceptance criteria for these results specified in the STP is that the MODFLOW-2000 produced solution for drawdown in this test shall be:

* within one percent of the analytic solution for all nodes between the pumping node and 1000 m distance from the pumping well at both 5 and 10 days after pumping commences
* within five percent of the analytic solution for all nodes between the pumping node and 5000 m distance from the pumping well at both 5 and 10 days after pumping commences

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Figure 1. Analytic Solution to Theis Drawdown Problem (MF‑ATC‑1)

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Figure 2. MODFLOW-2000 Results for Theis Drawdown Problem (MF‑ATC‑1; Single Precision)

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Figure 3. MODFLOW-2000 Results for Theis Drawdown Problem (MF‑ATC‑1; Double Precision)

The pumping well node was excluded from the test criteria because the solution in this node will clearly not be valid for comparison. Nodes beyond 10,000 meters distance from the pumping well will experience extremely small drawdown, and percent difference comparisons between such small numerical values will not be meaningful so these nodes were also excluded from the above criteria.

The validation spreadsheets “mf-atc-1\_mf2k-sp.xlsx” “mf-atc-1\_mf2k-sp.xlsx” were stored in the test directory \test-results. These spreadsheets include automatic determination of whether the above acceptance criteria were met. With regard to the above acceptance criteria at both pumping times (5 and 10 days) with the following measures were noted for the test on the Windows® operating system platform in Table 4.

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| Table 4. Test Results for MODFLOW-2000 with Advection-Diffusion Problem (MT-ATC-1) | | | | |
| **Maximum Distance from Pumping Well (m)** | **Pumping Time (d)** | **Maximum Percent Difference in Drawdown** | | **Pass/Fail** |
| **Single Precision** | **Double Precision** |
| *Criterion 1 (within one percent of the analytic solution for all nodes between the pumping node and 1000 m distance from the pumping well at both 5 and 10 days after pumping commences)* | | | | |
| 1000 m | 5 | 0.41 | 0.41 | PASS |
| 10 | 0.34 | 0.34 | PASS |
| *Criterion 2 (within five percent of the analytic solution for all nodes between the pumping node and 5000 m distance from the pumping well at both 5 and 10 days after pumping commences)* | | | | |
| 5000 m | 5 | 0.60 | 0.60 | PASS |
| 10 | 1.00 | 1.00 | PASS |
|  | | | | |

The same acceptance test was repeated on a Linux® platform to verify test results were comparable to drawdowns obtained on the Windows® platform. The calculated drawdowns were entered into spreadsheets “mf-atc-1\_mf2k-sp.xls” and “mf-atc-1\_mf2k-dp.xls” and the difference between drawdowns were calculated within these spreadsheets between those calculated in the Windows® tests and equivalent Linux® tests. This comparison showed insignificant numerical differences at several nodes for the single precision tests at 10 d (with a maximum drawdown difference 0.001 m) and no numerical differences for the double precision tests.

All results are within the acceptance criteria, and MODFLOW-2000 is therefore considered to pass this acceptance test.

The MODFLOW-2000 model input and output files were saved at completion of the test as well as the validation spreadsheet files, with exported results and computed differences, in the test directory. These files were then archived in the MODFLOW entry in MKS Integrity™ for preservation purposes.

### Test Results for MODFLOW-2000-MST

The logs maintained during the conduct of this test are provided in Attachment 3 for the Windows® testing and Attachment 4 for the Linux® testing. The expected results for drawdown with distance are those shown above for the baseline MODFLOW-2000 results.

The results were copied from the MODFLOW-2000-MST produced output list files named “mf-atc-1.lst” for drawdown at the respective times 5 and 10 days using a text editor program and pasted into directly to cells in the spreadsheet containing the analytical results. Graphically, the comparison of solutions is provided in the plots in Figure 4 for single-precision tests. For the double-precision tests, the results appear in Figure 5.

The acceptance criteria for these results specified in the STP is that the MODFLOW produced solution for drawdown in this test shall be:

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Figure 4. MODFLOW-2000-MST Results for Theis Drawdown Problem (MF‑ATC‑1; Single Precision)

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Figure 5. MODFLOW-2000-MST Results for Theis Drawdown Problem (MF‑ATC‑1; Double Precision)

* within one percent of the analytic solution for all nodes between the pumping node and 1000 m distance from the pumping well at both 5 and 10 days after pumping commences
* within five percent of the analytic solution for all nodes between the pumping node and 5000 m distance from the pumping well at both 5 and 10 days after pumping commences

The pumping well node was excluded from the test criteria because the solution in this node will clearly not be valid for comparison. Nodes beyond 5000 meters distance from the pumping well will experience extremely small drawdown, and percent difference comparisons between such small numerical values will not be meaningful so these nodes were also excluded from the above criteria.

The validation spreadsheets “mf-atc-1\_mf2k-mst-sp.xlsx” and “mf-atc-1\_mf2k-mst-dp.xlsx” include automatic determination of whether the above acceptance criteria were met. With regard to the above acceptance criteria at both pumping times (5 and 10 days) with the following measures were noted in Table 5.

The same acceptance test was repeated on a Linux® platform to verify test results were comparable to drawdowns obtained on the Windows® platform. The calculated drawdowns were entered into spreadsheets “mf-atc-1\_mf2k-mst-sp.xlsx” and “mf-atc-1\_mf2k-mst-dp.xlsx” and the difference between drawdowns were calculated within these spreadsheets between those calculated in the Windows® tests and equivalent Linux® tests, with results shown in Table 6. Thus, with regard to using Linux® versus Windows® platforms, these tests rendered nearly numerically identical results to the number of significant figures reported in the list files for single precision tests and numerically identical results for double precision tests.

These results all are within the acceptance criteria, and MODFLOW-2000-MST is therefore considered to pass this acceptance test.

The MODFLOW-2000-MST model input and output files were saved at completion of the test as well as the verification and validation spreadsheet files, with exported results and computed differences, in the test directory. These files were then archived in the MODFLOW entry in MKS Integrity™ for preservation purposes.

MODFLOW-2000-MST includes additional solvers of interest for use at Hanford. To test the solvers of interest included in the MST package, the test problem was repeated after reconfiguring the copied test case input files and results checked as for the SIP solver above. The additional solvers tested were Preconditioned Conjugate Gradient Nonlinear (PCGN), ORTHOMIN, Generalized Conjugate Gradient (GCG), and Generalized Minimal Residual (GMR) solvers. Testing of these additional solvers was performed using the single- and double- precision executable files on the Windows testing platform. The results of retesting using test problem MF-ATC-1 are summarized for the PCGN solver in Table 7, for the ORTHOMIN solver in Table 8, for the GCG solver in Table 9, and for the GMRES solver in Table 10, which indicate test results obtained using these two solvers met the criteria as well.

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| Table 5. Test Results for MODFLOW-2000-MST with Advection-Diffusion Problem (MT-ATC-1, SIP Solver) | | | | |
| **Maximum Distance from Pumping Well (m)** | **Pumping Time (d)** | **Maximum Percent Difference in Drawdown** | | **Pass/Fail** |
| **Single Precision** | **Double Precision** |
| *Criterion 1 (within one percent of the analytic solution for all nodes between the pumping node and 1000 m distance from the pumping well at both 5 and 10 days after pumping commences)* | | | | |
| 1000 m | 5 | 0.41 | 0.41 | PASS |
| 10 | 0.34 | 0.34 | PASS |
| *Criterion 2 (within five percent of the analytic solution for all nodes between the pumping node and 5000 m distance from the pumping well at both 5 and 10 days after pumping commences)* | | | | |
| 5000 m | 5 | 0.60 | 0.60 | PASS |
| 10 | 1.00 | 1.00 | PASS |

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| Table 6. Check of Numerical Differences in Drawdown between Windows® and Linux® Executable Files for MODFLOW-MST | | |
| Pumping Time (d) | Single Precision | Double Precision |
| 5 | Differences at 5 locations  (maximum difference: 1.0×10‑4 m) | No numerical differences |
| 10 | Differences at 4 locations  (maximum difference: 1.0×10‑3 m) | No numerical differences |
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| Table 7. Test Results for MODFLOW-2000-MST with Advection-Diffusion Problem (MT-ATC-1, PCGN Solver) | | | | |
| **Maximum Distance from Pumping Well (m)** | **Pumping Time (d)** | **Maximum Percent Difference in Drawdown** | | **Pass/Fail** |
| **Single Precision** | **Double Precision** |
| *Criterion 1 (within one percent of the analytic solution for all nodes between the pumping node and 1000 m distance from the pumping well at both 5 and 10 days after pumping commences)* | | | | |
| 1000 m | 5 | 0.99 | 0.99 | PASS |
| 10 | 0.82 | 0.81 | PASS |
| *Criterion 2 (within five percent of the analytic solution for all nodes between the pumping node and 5000 m distance from the pumping well at both 5 and 10 days after pumping commences)* | | | | |
| 5000 m | 5 | 2.24 | 2.24 | PASS |
| 10 | 2.11 | 2.11 | PASS |
|  | | | | |
| Table 8. Test Results for MODFLOW-2000-MST with Advection-Diffusion Problem (MT-ATC-1, ORTHOMIN Solver) | | | | |
| **Maximum Distance from Pumping Well (m)** | **Pumping Time (d)** | **Maximum Percent Difference in Drawdown** | | **Pass/Fail** |
| **Single Precision** | **Double Precision** |
| *Criterion 1 (within one percent of the analytic solution for all nodes between the pumping node and 1,000 m distance from the pumping well at both 5 and 10 days after pumping commences)* | | | | |
| 1000 m | 5 | 0.99 | 0.99 | PASS |
| 10 | 0.82 | 0.82 | PASS |
| *Criterion 2 (within five percent of the analytic solution for all nodes between the pumping node and 5000 m distance from the pumping well at both 5 and 10 days after pumping commences)* | | | | |
| 5000 m | 5 | 2.24 | 2.24 | PASS |
| 10 | 2.11 | 2.11 | PASS |
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| Table 9. Test Results for MODFLOW-2000-MST with Advection-Diffusion Problem (MT-ATC-1, GCG Solver) | | | | |
| **Maximum Distance from Pumping Well (m)** | **Pumping Time (d)** | **Maximum Percent Difference in Drawdown** | | **Pass/Fail** |
| **Single Precision** | **Double Precision** |
| *Criterion 1 (within one percent of the analytic solution for all nodes between the pumping node and 1,000 m distance from the pumping well at both 5 and 10 days after pumping commences)* | | | | |
| 1000 m | 5 | 0.99 | 0.99 | PASS |
| 10 | 0.82 | 0.82 | PASS |
| *Criterion 2 (within five percent of the analytic solution for all nodes between the pumping node and 5000 m distance from the pumping well at both 5 and 10 days after pumping commences)* | | | | |
| 5000 m | 5 | 2.24 | 2.24 | PASS |
| 10 | 2.11 | 2.11 | PASS |
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| Table 10. Test Results for MODFLOW-2000-MST with Advection-Diffusion Problem (MT-ATC-1, GMRES Solver) | | | | |
| **Maximum Distance from Pumping Well (m)** | **Pumping Time (d)** | **Maximum Percent Difference in Drawdown** | | **Pass/Fail** |
| **Single Precision** | **Double Precision** |
| *Criterion 1 (within one percent of the analytic solution for all nodes between the pumping node and 1,000 m distance from the pumping well at both 5 and 10 days after pumping commences)* | | | | |
| 1000 m | 5 | 0.99 | 0.99 | PASS |
| 10 | 0.82 | 0.82 | PASS |
| *Criterion 2 (within five percent of the analytic solution for all nodes between the pumping node and 5000 m distance from the pumping well at both 5 and 10 days after pumping commences)* | | | | |
| 5000 m | 5 | 2.24 | 2.24 | PASS |
| 10 | 2.11 | 2.11 | PASS |

### Test Results for MODFLOW-USG

The logs maintained during the conduct of this test are provided in Attachment 9 for the Windows® testing and Attachment 10 for the Linux® testing. The expected results for drawdown with distance are those shown above for the baseline MODFLOW-2000 results.

The MODFLOW-USG Sparse Matrix Solver (SMS) package include two solvers: the *χ*MD solver, an asymmetric sparse matrix solver, and the unstructured pre-conditioned conjugate gradient (PCGU) solver. The results were copied from the MODFLOW-USG produced output list files named “theis.lst” for drawdown at the respective times 5 and 10 days using a text editor program and pasted into directly to cells in the spreadsheet containing the analytical results.

Graphically, the comparison of solutions is provided in the plots in Figure 6 for single-precision tests with the *χ*MD solver. For the double-precision tests, the results appear in Figure 7.

The acceptance criteria for these results specified in the STP is that the MODFLOW produced solution for drawdown in this test shall be:

* within one percent of the analytic solution for all nodes between the pumping node and 1000 m distance from the pumping well at both 5 and 10 days after pumping commences
* within five percent of the analytic solution for all nodes between the pumping node and 5000 m distance from the pumping well at both 5 and 10 days after pumping commences

The pumping well node was excluded from the test criteria because the solution in this node will clearly not be valid for comparison. Nodes beyond 5000 meters distance from the pumping well will experience extremely small drawdown, and percent difference comparisons between such small numerical values will not be meaningful so these nodes were also excluded from the above criteria.

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Figure 6 MODFLOW-USG Results for Theis Drawdown Problem (MF‑ATC‑1; Single Precision, *χ*MD Solver)

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Figure 7 MODFLOW-USG Results for Theis Drawdown Problem (MF‑ATC‑1; Double Precision, *χ*MD Solver)

The validation spreadsheets “mf-atc-1\_mfusg-sp.xlsx” and “mf-atc-1\_mfusg-dp.xlsx” include automatic determination of whether the above acceptance criteria were met. With regard to the above acceptance criteria at both pumping times (5 and 10 days) with the following measures were noted in Table 11.

The same acceptance test was repeated on a Linux® platform to verify test results were comparable to drawdowns obtained on the Windows® platform. The calculated drawdowns were entered into spreadsheets “mf-atc-1\_mfusg-sp.xlsx” and “mf-atc-1\_mfusg-dp.xlsx” and the difference between drawdowns were calculated within these spreadsheets between those calculated in the Windows® tests and equivalent Linux® tests, with results shown in Table 12. Thus, with regard to using Linux® versus Windows® platforms, these tests rendered numerically identical results to the number of significant figures reported in the list files for the single and double precision tests.

These results all are within the acceptance criteria, and MODFLOW-USG is therefore considered to pass this acceptance test. For the Linux® compilation, the Intel® Fortran Compiler version 13.0.1 was used.

The MODFLOW-USG model input and output files were saved at completion of the test as well as the verification and validation spreadsheet files, with exported results and computed differences, in the test directory. These files were then archived in the MODFLOW entry in MKS Integrity™ for preservation purposes.

To test the solvers included in the SMS package, the test problem was repeated after reconfiguring the copied test case input files and results checked as for the above for the additional solver (PCGU) using the single- and double precision executable files on the Windows testing platform. The results of the additional testing with the PCGU solver using test problem MF-ATC-1 are summarized in Table 13 that indicates test results obtained using the PCGU solver did not met the acceptance criteria initially. Specifically, the solution was not within one percent of the analytic solution for all nodes between the pumping node and 1000 m distance from the pumping well at 5 days. The convergence criteria for head closure (variable HCLOSE) for the test case was 1.00E-03 meters. To test the sensitivity of HCLOSE to the solution meeting the acceptance criteria, HCLOSE was decreased an order of magnitude and the solution was found meet the acceptance criteria.

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| Table 11. Test Results for MODFLOW-USG for Theis Drawdown Problem Problem (MT-ATC-1, χMD Solver) | | | | |
| **Maximum Distance from Pumping Well (m)** | **Pumping Time (d)** | **Maximum Percent Difference in Drawdown** | | **Pass/Fail** |
| **Single Precision** | **Double Precision** |
| *Criterion 1 (within one percent of the analytic solution for all nodes between the pumping node and 1000 m distance from the pumping well at both 5 and 10 days after pumping commences)* | | | | |
| 1000 m | 5 | 0.99 | 0.99 | PASS |
| 10 | 0.82 | 0.82 | PASS |
| *Criterion 2 (within five percent of the analytic solution for all nodes between the pumping node and 5000 m distance from the pumping well at both 5 and 10 days after pumping commences)* | | | | |
| 5000 m | 5 | 2.24 | 2.24 | PASS |
| 10 | 2.11 | 2.11 | PASS |

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| Table 12. Check of Numerical Differences in Drawdown between Windows® and Linux® Executable Files for MODFLOW-USG with *χ*MD Solver | | |
| **Pumping Time (d)** | **Single Precision** | **Double Precision** |
| 5 | No numerical differences | No numerical differences |
| 10 | No numerical differences | No numerical differences |
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| Table 13. Test Results for MODFLOW-USG for Theis Drawdown Problem (MT-ATC-1, PCGU Solver) | | | | |
| **Maximum Distance from Pumping Well (m)** | **Pumping Time (d)** | **Maximum Percent Difference in Drawdown** | | **Pass/Fail** |
| **Single Precision** | **Double Precision** |
| *Criterion 1 (within one percent of the analytic solution for all nodes between the pumping node and 1000 m distance from the pumping well at both 5 and 10 days after pumping commences)* | | | | |
| 1000 m | 5 | 1.03 | 1.03 | FAIL HCLOSE = 1.0E-03  PASS HCLOSE=1.0E-04 1 |
| 10 | 0.82 | 0.82 | PASS |
| *Criterion 2 (within five percent of the analytic solution for all nodes between the pumping node and 5000 m distance from the pumping well at both 5 and 10 days after pumping commences)* | | | | |
| 5000 m | 5 | 2.26 | 2.26 | PASS |
| 10 | 2.15 | 2.15 | PASS |
| 1. Test results obtained using the PCGU solver did not met the acceptance criteria initially. The convergence criteria for head closure (variable HCLOSE) for the test case was 1.00E-03 meters. However, when HCLOSE was decreased an order of magnitude, the solution met the acceptance criteria. | | | | |

## **MT-ATC-1: van Genuchten and Alves Advection-Diffusion Problem**

This test is designed to validate contaminant transport by means of a calculation of advection and diffusion in a uniform flow field in a porous medium. The results of the solution obtained using he MT3DMS code are to be compared to the solution presented by van Genuchten and Alves (1982). Details of this test, the basis for the analytical solution, and expected results are presented in the STP.

### Test Results for MT3DMS

The logs maintained during the conduct of this test are provided in Attachment 5 for the Windows® testing and Attachment 6 for the Linux® testing. The expected results for concentration with distance were calculated from the analytical solution for 2400 and 9600 days of transport in validation spreadsheets mt-atc-1\_mt3d-dp-2400d.xlsx” and “mt-atc-1\_mt3d-dp-9600d.xlsx”, respectively, and appear graphically in Figure 8.

The concentration results were copied from the MT3DMS-produced output list file “mt‑atc‑1.m3d” at the respective solution times 2400 and 9600 days using a text editor program and pasted into directly to cells in the spreadsheets “mt-atc-1\_mt3d-sp-2400d.xlsx” and “mt-atc-1\_mt3d-sp-9600d.xlsx”, respectively for the single-precision executable tests, that contain the analytical solution to this problem. Spreadsheets “mt-atc-1\_mt3d-dp-2400d.xlsx” and “mt-atc-1\_mt3d-dp-9600d.xlsx”, are used for the double-precisions tests. Graphically, the comparison of solutions for the single precision executable is provided in the plots in Figure 9. The results for the double precision executable are similar, as shown in Figure 10.

The acceptance criteria for this test are that the MT3DMS solution for concentration in this test shall:

* Criterion 1 - match the peak concentration distance to within 1 m at both 2400 days and 9600 days simulation time
* Criterion 2 – the peak concentration will be within one percent of the analytical value at both 2400 days and 9600 days simulation time.

Criterion 1 gives evidence that the advection component is valid while criterion 2 provides evidence that the dispersion component is valid. The validation spreadsheets “mt-atc-1\_mt3d-sp-2400d.xlsx” and “mt-atc-1\_mt3d-sp-9600d.xlsx” include automatic determination of whether the above acceptance criteria are met for the single precision executable files, and similarly “mt-atc-1\_mt3d-dp-2400d.xlsx” and “mt-atc-1\_mt3d-dp-9600d.xlsx” for the double precision executable files. With regard to the above acceptance criteria at both transport times (2400 and 9600 days) with the results shown in Table 14.

All of the above results were identical for both the single and the double precision tests. These all are within the acceptance criteria, and MT3DMS is therefore considered to pass this acceptance test.

The same acceptance test was repeated on a Linux® platform to verify test results were comparable to concentrations obtained on the Windows® platform. The calculated concentrations were entered into the validation spreadsheets as well and the difference

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Figure 8. Analytic Solution to van Genuchten and Alves Advection-Dispersion Problem (MT‑ATC‑1)

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Figure 9. MT3DMS Solution to van Genuchten and Alves Advection-Dispersion Problem (MT‑ATC‑1; Single Precision)

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Figure 10. MT3DMS Solution to van Genuchten and Alves Advection-Dispersion Problem (MT‑ATC-1; Double Precision)

| Table 14. MT3DMS Test Results for van Genuchten and Alves Advection-Diffusion Problem (MT-ATC-1) | | | | |
| --- | --- | --- | --- | --- |
| **Solution Time (d)** | **Analytic Solution** | **MT3DMS Solution1** | **Difference** | **Pass/Fail** |
| *Criterion 1 (peak concentration location)* | | | | |
| 2400 | *Cmax* at 3200 m | *Cmax* in grid cell from 3200 to 3300 m (cell center 3250 m) | 0 | PASS |
| 9600 | *Cmax* at 6800 m | *Cmax* in grid cell from 6800 m to 6900 m (cell center at 6850 m) | 0 | PASS |
| *Criterion 2 (peak relative concentration C/C0)* | | | | |
| 2400 | *C/C0 =* 0.7793 | *C/C0 =* 0.7759 | 0.00343 (0.440%) | PASS |
| 9600 | *C/C0 =* 0.4597 | *C/C0 =*0.4583 | 0.00141 (0.306%) | PASS |
| 1 Solution identical for single- and double-precision executable files. | | | | |

between drawdowns were calculated within these spreadsheets between those calculated in the Windows® tests and equivalent Linux® tests. This comparison is shown in Table 15.

No numerical differences were detected within the reporting limits of the .m3d output files between the Windows® and Linux® versions of these executable files for the same tests problems.

The MODFLOW and MT3DMS model input and output files for this test were saved at completion of the test as well as the Excel validation spreadsheet files, with exported results and computed differences, in the test directory. These files were then archived in the MODFLOW entry in MKS Integrity™ for preservation purposes.

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| Table 15. Check of Numerical Differences in Drawdown between Windows® and Linux® Executable Files | | |
| Simulation Time (d) | Single Precision | Double Precision |
| 2400 | No Numerical Differences | No Numerical Differences |
| 9600 | No Numerical Differences | No Numerical Differences |

### Test Results for MT3DMS-MST

The logs maintained during the conduct of this test are provided in Attachment 7 for the Windows® testing and Attachment 8 for the Linux® testing. The expected results for concentration with distance were calculated from the analytical solution for 2400 and 9600 days of transport in validation spreadsheets mt-atc-1\_mt3d-mst-dp-2400d.xlsx” and “mt-atc-1\_mt3d-mst-dp-9600d.xlsx”, respectively, and appear graphically in Figure 11.

The concentration results were copied from the MT3DMS-produced output list file “mt‑atc‑1.m3d” at the respective solution times 2400 and 9600 days using a text editor program and pasted into directly to cells in the spreadsheets mt-atc-1\_mt3d-mst-sp-2400d.xlsx” and “mt-atc-1\_mt3d-mst-sp-9600d.xlsx”, respectively for the single-precision executable tests, that contain the analytical solution to this problem. Spreadsheets mt-atc-1\_mt3d-mst-dp-2400d.xlsx” and “mt-atc-1\_mt3d-mst-dp-9600d.xlsx”, are used for the double-precisions tests. Graphically, the comparison of solutions for the single precision executable is provided in the plots in Figure 12. The results for the double precision executable are similar, as shown in Figure 13.

The acceptance criteria for this test are that the MT3DMS solution for concentration in this test shall:

* Criterion 1 - match the peak concentration distance to within 1 m at both 2400 days and 9600 days simulation time
* Criterion 2 – the peak concentration will be within one percent of the analytical value at both 2400 days and 9600 days simulation time.

Criterion 1 gives evidence that the advection component is valid while criterion 2 provides evidence that the dispersion component is valid. The validation spreadsheets include automatic determination of whether the above acceptance criteria are met. With regard to the above

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Figure 11. Analytic Solution to van Genuchten and Alves Advection-Dispersion Problem (MT‑ATC‑1)

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Figure 12. MT3DMS-MST Solution to van Genuchten and Alves Advection-Dispersion Problem (MT‑ATC‑1; Single Precision)

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Figure 13. MT3DMS-MST Solution to van Genuchten and Alves Advection-Dispersion Problem (MT‑ATC-1; Double Precision)

acceptance criteria at both transport times (2400 and 9600 days) with the results shown in Table 16.

All of the above results were identical for both the single and the double precision tests. These all are within the acceptance criteria, and MT3DMS is therefore considered to pass this acceptance test.

The same acceptance test was repeated on a Linux® platform to verify test results were comparable to concentrations obtained on the Windows® platform. The calculated concentrations were entered into a new space in the validation spreadsheets and the difference between drawdowns were calculated within these spreadsheets between those calculated in the Windows® tests and equivalent Linux® tests. This comparison is shown in Table 17. No numerical differences were detected within the reporting limits of the .m3d output files between the Windows® and Linux® versions of these executable files for the same tests problems.

The MODFLOW and MT3DMS model input and output files for this test were saved at completion of the test as well as the Excel validation spreadsheet files, with exported results and computed differences, in the test directory. These files were then archived in the MODFLOW entry in MKS Integrity™ for preservation purposes.

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| Table 16. Test Results for van Genuchten and Alves Advection-Diffusion Problem (MT-ATC-1) | | | | |
| **Solution Time (d)** | **Analytic Solution** | **MT3DMS-MST Solution1** | **Difference** | **Pass/Fail** |
| *Criterion 1 (peak concentration location)* | | | | |
| 2400 | *Cmax* at 3200 m | *Cmax* in grid cell from 3200 to 3300 m (cell center 3250 m) | 0 | PASS |
| 9600 | *Cmax* at 6800 m | *Cmax* in grid cell from 6800 m to 6900 m (cell center at 6850 m) | 0 | PASS |
| *Criterion 2 (peak relative concentration C/C0)* | | | | |
| 2400 | *C/C0 =* 0.7793 | *C/C0 =* 0.7759 | 0.00343 (0.440%) | PASS |
| 9600 | *C/C0 =* 0.4597 | *C/C0 =* 0.4583 | 0.00141 (0.306%) | PASS |
| 1 Solution identical for single- and double-precision executable files. | | | | |

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| Table 17. Check of Numerical Differences in Drawdown between Windows® and Linux® Executable Files | | |
| Simulation Time (d) | Single Precision | Double Precision |
| 2400 | No Numerical Differences | No Numerical Differences |
| 9600 | No Numerical Differences | No Numerical Differences |

## Comprehensive Assessment

The test plan intentionally did not exhaustively test all the features and modules of MODFLOW-2000, MODFLOW-2000-MST, MT3DMS, and MT3DMS-MST; such a testing program would be prohibitive in terms of schedule, scope, and budget. Instead, test problems were devised to demonstrate applicability of these software tools with respect to critical processes that will be simulated for Hanford problems, with emphasis on groundwater flow, pumping, boundary conditions, and drawdown for aquifer properties representative of those found at the Hanford Site.

Test and documentation time requirements are as follows for the builds to date:

* Build 1 (November 2009) 3 days
* Build 2 (March 2010), 1 day
* Build 3 (May 2010),½ day
* Build 4 (November 2010), 1 day
* Build 5 (March 2012), 3 days
* Build 6 (May 2012), 2 days
* Build 7 (March 2015), 4 days
* Build 7 (May 2015, MODFLOW-USG only), 3 days
* Build 8 (November 2015, current),

Computer resource utilization for model runs with MODFLOW and MT3DMS codes was minimal for all of these tests.

## Incident Reporting

The following incident was encountered in conducting the acceptance tests for CHPRC Build 8 of this software:

* In preparing Linux® executable files, some compilation issues were encountered for MT3DMS-MST these errors were debugged, corrections identified, and the vendor (SSP&A) notified. SSP&A corrected the issues and resubmitted the package before acceptance testing resumed. All problems identified were resolved in the resubmitted code.

The following incident was encountered in testing MODFLOW-USG in Build 7, and remains unchanged in Build 8:

* With the PCGU solver and the test case HCLOSE value of 1.0E-3 meters, the acceptance criteria was not met. Adjusting HCLOSE to 1.0E-4 meters resulted in meeting the acceptance criteria.

There are no unresolved incidents and no impact on placing this software into operation.

# REFERENCES

CHPRC-00259, 2014, *MODFLOW and Related Codes Software Test Plan*, Rev. 3, CH2M HILL Plateau Remediation Company, Richland, Washington.

Theis, CV, 1935, “The Relation between the Lowering of the Piezometric Surface and the Rate and Duration of Discharge of a Well using Ground-water Storage,” Transactions American Geophysical Union, Vol. 16, pg.519-524.

van Genuchten, MT, and WJ Alves, 1982, *Analytical Solutions of the One-Dimensional Convective-Dispersive Solute Transport Equation*, ARS Technical Bulletin 1661, U.S. Department of Agriculture.

**Acronyms, Abbreviations, and Definitions**

| Acronym | Description |
| --- | --- |
| ATR | Acceptance Test Report |
| CHPRC | CH2M HILL Plateau Remediation Company |
| MKS Integrity™ | configuration management system software |
| MODFLOW | MODular three-dimensional finite-difference ground-water FLOW model (software) |
| MT3DMS | modular three-dimensional, multi-species transport model for simulation of advection, dispersion, and chemical reactions of contaminants in groundwater systems (software) |
| MST | Minimum saturated thickness (code enhancements to MODFLOW 2000 and MT3DMS to improve handling of grid cells saturation/desaturation) |
| SMP | Software Management Plan |
| SSP&A | S.S. Papadopulos and Associates |
| STP | Software Test Plan |
| USGS | U.S. Geological Survey |

# ATTACHMENTS

# Completed Test Log: MODFLOW Acceptance Test Case 1 (MF-ATC-1): MODFLOW-2000 Executable Files for Windows® Operating System

1. Completed Test Log: MODFLOW Acceptance Test Case 1 (MF-ATC-1): MODFLOW-2000 Executable Files for Linux® Operating System
2. Completed Test Log: MODFLOW Acceptance Test Case 1 (MF-ATC-1): MODFLOW-2000-MST Executable Files for Windows® Operating System
3. Completed Test Log: MODFLOW Acceptance Test Case 1 (MF-ATC-1): MODFLOW-2000-MST Executable Files for Linux® Operating System
4. Completed Test Log: MT3DMS Acceptance Test Case 1 (MT-ATC-1): MT3DMS Executable Files for Windows® Operating System
5. Completed Test Log: MT3DMS Acceptance Test Case 1 (MT-ATC-1): MT3DMS Executable Files for Linux® Operating System
6. Completed Test Log: MT3DMS Acceptance Test Case 1 (MT-ATC-1): MT3DMS-MST Executable Files for Windows® Operating System
7. Completed Test Log: MT3DMS Acceptance Test Case 1 (MT-ATC-1) for MT3DMS-MST Executable Files for Linux® Operating System
8. Completed Test Log: MODFLOW Acceptance Test Case 1 (MF-ATC-1): MODFLOW-USG Executable Files for Windows® Operating System
9. Completed Test Log: MODFLOW Acceptance Test Case 1 (MF-ATC-1): MODFLOW-USG Executable Files for Linux® Operating System

ATTACHMENT 1

Completed Test Log: MODFLOW Acceptance Test Case 1 (MF-ATC-1): MODFLOW-2000 Executable Files for Windows® Operating System

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| MODFLOW Acceptance Test Case 1  Description: Theis Transient Drawdown Problem | | | Test Case #:  MF-ATC-1 | Date:  4 Mar 2015 |
| System Attributes:  Version #: MODFLOW-2000  Release #: CHPRC Build 8 (Identical to Build 6)  Environment: Windows 7® Enterprise SP1  Server: WF22668 | | | Test Performed by:  William E. Nichols, CHPRC  [Signed in Previous Revision 6 to this document] | |
| Test Step # | Requirement # | Test Instruction | Expected Result | Actual Result |
| 1 | Obtain source code or executable for MODFLOW-2000-MST code from software owner & install on target computer | Compile using appropriate Fortran compiler, if necessary | MODFLOW executable is ready and functional | Copied source code obtained from USGS website and archived in MKS Integrity™ to computer WC95463.  Updated “build” batch files to compile and link all necessary code to build the executable files for single and double precision (build-lahey-sp.bat and build-lahey-dp.bat):   * Compiles all C source code using Fujitsu C (fcc) compiler * Compiles all Fortran source code using Lahey/Fujitsu Fortran (Release 7.20) for Windows® compiler * Links all object files with required library statically   Invoked these “build” batch files to compile and link the single- and double-precision executable for Windows. The compilation and link returned no errors.  Executable files copied to directory …\bin (with local PATH variable assigned) as executable files mf2k-chprc07spl.exe and mf2k-chprc07dpl.exe. |
| 2 | Obtain files for test problem from software owner | Copy files to appropriate test directory | Test files are ready for use | Test files obtained from MKS Integrity™ for acceptance test case MF-ATC-1. Copied to test directory on external hard drive in directory:  …\test\MODFLOW\Build-7  Subdirectories:  \mf-atc-1\_dp (double precision test)  \mf-atc-1\_sp (single precision test) |
| 3 | Run MODFLOW to solve for flow problem | Execute MODFLOW against mf-atc-1.nam name file in test directory | MODFLOW executes without error | While logged onto WF22668 as a user without administrator privileges, executed mf2k-chprc07spl.exe and mf2k‑chprc07dpl.exe successfully for both pumping durations problems (in test subdirectories /pumping-05-d and /pumping-10-d). |
| 4 | Extract results and transfer to validation spreadsheet | Using a text editor, copy MODFLOW-calculated drawdown values from end of list file mf-atc-1.lis and paste into appropriate cells in validation spreadsheet “mt-atc-1.xlsx” | Spreadsheet will update tables, graphics, and acceptance test results | Used a text editor program to open the THEIS.LIS file for each pumping duration case and copy the drawdowns for the first row of results, representing the radial drawdown results. Pasted these results into the respective worksheets of validation spreadsheets “mf-atc-1\_mf2k-sp.xlsx” and “mf-atc-1\_mf2k-dp.xlsx” (separate copy of this spreadsheet for testing single and double precision versions, kept in appropriate testing subdirectories). |
| 5 | Use test results and graphics from spreadsheet to complete test reporting in ATR | Copy and paste graphics and note acceptance test results in ATR | MODFLOW acceptance test criterion are met | Copied and pasted resulting graphics to the acceptance test report to show comparison of analytic and MODFLOW results; noted results in ATR for acceptance criteria calculated in copies the spreadsheets “mf-atc-1\_mf2k-sp.xlsx” and “mf-atc-1\_mf2k-dp.xlsx” for each repeated test by precision.  All criteria were met for this software.  Test directory contents were committed to MKS Integrity© for this test. |

ATTACHMENT 2

Completed Test Log: MODFLOW Acceptance Test Case 1 (MF-ATC-1): MODFLOW-2000 Executable Files for Linux® Operating System

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| MODFLOW Acceptance Test Case 1  Description: Theis Transient Drawdown Problem | | | Test Case #:  MF-ATC-1 | Date:  3 Mar 2015 |
| System Attributes:  Version #: MODFLOW-2000  Release #: CHPRC Build 8 (Identical to Build 6)  Environment:: Redhat Enterprise Linux® release 5.8  Server: Tellus Linux® Cluster | | | Test Performed by:  William E. Nichols, CHPRC  [Signed in Previous Revision 6 to this document] | |
| Test Step # | Requirement # | Test Instruction | Expected Result | Actual Result |
| 1 | Obtain source code or executable for MODFLOW-2000-MST code from software owner & install on target computer | Compile using appropriate Fortran compiler, if necessary | MODFLOW executable is ready and functional | Copied source code obtained from USGS website and archived in MKS Integrity™ to Tellus Linux® Cluster.  Developed “build-lahey-sp.sh” and “build-lahey-dp.sh”, to compile and link all necessary code to build the software executable files:   * Compiles all C source code using GNU C (gcc) compilerCompiles all Fortran source code using Lahey Fortran Compiler for Linux® Release 8.01b compiler * Links all object files with required library statically   Code executable files are placed in executable test …/bin-test for testing and were named mf2k-chprc07spl.x and mf2k-chprc07dpl.x. |
| 2 | Obtain files for test problem from software owner | Copy files to appropriate test directory | Test files are ready for use | Files obtained from MKS Integrity™ for acceptance test case MF-ATC-1. Placed in directory …/src/modflow/build-7/modflow in appropriate subdirectories to separately test single and double precision executable files. |
| 3 | Run MODFLOW to solve for flow problem | Execute MODFLOW against mf-atc-1.nam name file in test directory | MODFLOW executes without error | Logged onto Tellus as a user that does not have administrator privileges.  Executed mt2k-chprc07spl.x and mf2k-chprc07dpl.x successfully for both pumping durations (in subdirectories /pumping-05-d and /pumping-10-d) for both precision level tests. |
| 4 | Extract results and transfer to validation spreadsheet | Using a text editor, copy MODFLOW-calculated drawdown values from end of list file mf-atc-1.lis and paste into appropriate cells in validation spreadsheet “mt-atc-1.xlsx” | Spreadsheet will update tables, graphics, and acceptance test results | Used text editor program to open the THEIS.LIS file for each pumping duration case and copy the drawdowns for the first row of results, representing the radial drawdown results. Pasted these results into the respective worksheets of Excel® validation spreadsheets “mf-atc-1-sp.xlsx” and “mf-atc-1-dp.xlsx” (separate copy of this spreadsheet for testing single and double precision versions, kept in appropriate testing subdirectories). |
| 5 | Use test results and graphics from spreadsheet to complete test reporting in ATR | Copy and paste graphics and note acceptance test results in ATR | MODFLOW acceptance test criterion are met | Copy and pasted resulting graphics to the acceptance test report to show comparison of analytic and MODFLOW results; noted results in ATR for acceptance criteria calculated in copies the spreadsheets “m mf-atc-1\_mf2k-sp.xlsx and “mf-atc-1\_mf2k-dp.xlsx” for each repeated test by precision.  All criteria were met for this software.  Test directory contents were committed to MKS Integrity© for this test. |

ATTACHMENT 3

Completed Test Log: MODFLOW Acceptance Test Case 1 (MF-ATC-1): MODFLOW-2000-MST Executable Files for Windows® Operating System

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| MODFLOW Acceptance Test Case 1  Description: Theis Transient Drawdown Problem | | | Test Case #:  MF-ATC-1 | Date:  4 Mar 2015 |
| System Attributes:  Version #: MODFLOW-2000-MST  Release #: CHPRC Build 8 (Identical to Build 6)  Environment: Windows 7® Enterprise SP1  Server: WF22668 | | | Test Performed by:  William E. Nichols, CHPRC/INTERAJoan Blainey, INTERA  [Signed in Previous Revision 6 to this document] | |
| Test Step # | Requirement # | Test Instruction | Expected Result | Actual Result |
| 1 | Obtain source code or executable for MODFLOW-2000-MST code from software owner & install on target computer | Compile using appropriate Fortran compiler, if necessary | MODFLOW executable is ready and functional | Source code and Windows® executable files obtained by download from SSP&A FTP site on 19-Feb-2015 were archived in MKS Integrity™ (2517). Executable files was then ported to target computer and placed in c:\bin directory. |
| 2 | Obtain files for test problem from software owner | Copy files to appropriate test directory | Test files are ready for use | Files obtained from MKS Integrity™ for acceptance test case MF-ATC-1; and copied to directory  …\test\MODFLOW\Build-7\mf2k  in appropriate subdirectories for separately testing the single and double precision executable files. |
| 3 | Run MODFLOW to solve for flow problem | Execute MODFLOW against mf-atc-1.nam name file in test directory | MODFLOW executes without error | Logged onto WF22668 with a user account that does not have administrator privileges.  Successfully executed mt2k-mst-chprc07spv.exe and mt2k-mst-chprc07dpv.exe successfully for both pumping durations (in subdirectories /pumping-05-d and /pumping-10-d). |
| 4 | Extract results and transfer to validation spreadsheet | Using a text editor, copy MODFLOW-calculated drawdown values from end of list file mf-atc-1.lis and paste into appropriate cells in validation spreadsheet “mt-atc-1.xlsx” | Spreadsheet will update tables, graphics, and acceptance test results | Used text editor program to open the THEIS.LIS file for each pumping duration case and copy the drawdowns for the first row of results, representing the radial drawdown results. Pasted these results into the respective copies of the worksheets of Excel® validation spreadsheets “mf-atc-1\_mf2k-mst-sp.xlsx” for single precision results and “mf-atc-1\_mf2k-mst-dp.xlsx” for double precision results. |
| 5 | Use test results and graphics from spreadsheet to complete test reporting in ATR | Copy and paste graphics and note acceptance test results in ATR | MODFLOW acceptance test criterion are met | Copy and pasted resulting graphics to the acceptance test report to show comparison of analytic and MODFLOW results; noted results in ATR for acceptance criteria calculated in validation spreadsheets “mf-atc-1\_mf2k-mst-sp.xlsx” and “mf-atc-1\_mf2k-mst-dp.xlsx”.  All criteria were met for this software.  Test directory contents were committed to MKS Integrity© for this test. |

ATTACHMENT 4

Completed Test Log: MODFLOW Acceptance Test Case 1 (MF-ATC-1): MODFLOW-2000-MST Executable Files for Linux® Operating System

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| MODFLOW Acceptance Test Case 1  Description: Theis Transient Drawdown Problem | | | Test Case #:  MF-ATC-1 | Date:  3 Mar 2015 |
| System Attributes:  Version #: MODFLOW-2000-MST  Release #: CHPRC Build 8 (Identical to Build 6)  Environment:: Redhat Enterprise Linux® release 5.8  Server: Tellus Linux® Cluster | | | Test Performed by:  William E. Nichols, CHPRC  [Signed in Previous Revision 6 to this document] | |
| Test Step # | Requirement # | Test Instruction | Expected Result | Actual Result |
| 1 | Obtain source code or executable for MODFLOW-2000-MST code from software owner & install on target computer | Compile using appropriate Fortran compiler, if necessary | MODFLOW executable is ready and functional | Copied source code obtained by electronic mail in compressed archive form from SSP&A FTP site on 19-Feb-2015 was archived in MKS Integrity™ (2517) and placed in source directory on Tellus Linux® Cluster.  Developed build-lahey-sp.sh” and “build-lahey-sp.sh”, scripts to compile and link all necessary code to build the software executable files:   * Compiles all C source code using Gnu C for Linux compiler * Compiles all Fortran source code using Lahey Fortran Compiler for Linux® Release 8.01b compiler * Links all object files with required library statically   Build script places code executable files in CHPRC executables test directory …/bin-test and these are named mf2k-mst-chprc07spl.x and mf2k-mst-07chprcdpl.x for single and double precision executable files, respectively. |
| 2 | Obtain files for test problem from software owner | Copy files to appropriate test directory | Test files are ready for use | Copied acceptance test case file from MKS Integrity™ for acceptance test case MF-ATC-1 to directory …/test/modflow/build-7/mf2k in appropriate subdirectories for separately testing the single and double precision executable files. |
| 3 | Run MODFLOW to solve for flow problem | Execute MODFLOW against mf-atc-1.nam name file in test directory | MODFLOW executes without error | Logged onto Tellus with user account that does not have administrator privileges. Confirmed that the .bashrc file placed user in “test mode” with PATH variable pointing to executables in test executable directory /bin-test rather than production directory …/bin.  Successfully executed mt2k-mst-chprc07spl.x and mt2k-mst-chprc07dpl.x successfully for both pumping durations (in subdirectories /pumping-05-d and /pumping-10-d). |
| 4 | Extract results and transfer to validation spreadsheet | Using a text editor, copy MODFLOW-calculated drawdown values from end of list file mf-atc-1.lis and paste into appropriate cells in validation spreadsheet “mt-atc-1.xlsx” | Spreadsheet will update tables, graphics, and acceptance test results | Used text editor program to open the THEIS.LIS file for each pumping duration case and copy the drawdowns for the first row of results, representing the radial drawdown results. Pasted these results into new space in the respective copies of the worksheets of Excel® validation spreadsheets “mf-atc-1\_mf2k-mst-sp.xlsx” and “mf-atc-1\_mf2k-mst-dp.xlsx” for single- and double-precision results, respectively. Calculated differences in drawdown between the results from the Windows® test of this case and this run within the spreadsheets and noted differences where these occurred. |
| 5 | Use test results and graphics from spreadsheet to complete test reporting in ATR | Copy and paste graphics and note acceptance test results in ATR | MODFLOW acceptance test criterion are met | There were no differences compared to the test case results for the equivalent Windows® cases with one exception (single precision test for 5 days of pumping), and the differences in this case were determined to be numerically insignificant.  All criteria were met for this software.  Test directory contents were committed to MKS Integrity© for this test. |

ATTACHMENT 5

Completed Test Log: MT3DMS Acceptance Test Case 1 (MT-ATC-1): MT3DMS Executable Files for Windows® Operating System

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| --- | --- | --- | --- | --- | --- | --- |
| MT3DMS Acceptance Test Case 1  Description: One-Dimensional Advective-Diffusive Transport | | | | Test Case #:  MT-ATC-1 | | Date:  4 Mar 2015 |
| System Attributes:  Version #: MT3DMS  Release #: CHPRC Build 8 (Identical to Build 7)  Environment: Windows 7® Enterprise SP1  Server: WF22668 | | | | Test Performed by:  William E. Nichols, CHPRC  [Signed in Previous Revision 6 to this document] | | |
| Test Step # | Requirement # | Test Instruction | Expected Result | | Actual Result | |
| 1 | Obtain source code or executable for MODFLOW-2000-MST and MT3DMS code from software owner & install on target computer | Compile using appropriate Fortran compiler, if necessary | MODFLOW and MT3DMS executables are ready and functional | | For the flow solution used in this test, used the test installation of MODFLOW executable files mf2k-mst-chprc07spl.exe and mf2k-mst-chprc07dpl.exe that were prepared and tested in acceptance test (MF-ATC-1) logged in Attachment 2.  The source code for MT3DMS obtained by FTP download in compressed archive form from MT3DMS code maintenance site on 3-Feb-2015 was archived in MKS Integrity™ (2517). Batch files build-lahey-sp.bat and build-lahey-dp.bat were constructed to direct compilation and linking of executable files, named mt3d-chprc07spl.exe (single precision) and mt3d-chprc07dpl.exe (double precision).  Placed copies of these code executable files in directory …\bin. | |
| 2 | Obtain files for test problem from software owner | Copy files to appropriate test directory | Test files are ready for use | | Files obtained from MKS Integrity™ for acceptance test case MT-ATC-1 were obtained and placed in test directory:  …\test\MODFLOW\Build-7\mt3dms | |
| 3 | Run MODFLOW to solve for flow problem | Execute MODFLOW against mt-atc-1.nam name file in /flow test directory | MODFLOW executes without error; flow results transfer file is ready for use in next step | | Logged onto WF22668 as a user without administrator privileges. Set the PATH variable pointed to executable files in test directory …\bin\  Executed MODFLOW (mf2k-mst-chprc07spl.exe and mf2k-mst-chprc07dpl.exe) against steady-state flow solution case without error for single and double precision cases; flow results prepared in transfer file mt-atc-1.ftl. | |
| 4 | Run MT3DMS to solve for transport in both time durations | Execute MT3DMS against mt-atc-1.nam name file in both /transport\_2400d and /transport\_9600d subdirectories | MT3DMS executes without error; transport results are available in mt-atc-1.m3d in both time solution subdirectories | | MT3DMS executed without error for both 2400 day and 9600 day transport duration cases for both single and double precision executable files. | |
| 5 | Extract results and transfer to validation spreadsheets | Using a text editor, copy MT3DMS-calculated concentration values from end of list file mf-atc-1.m3d and paste into appropriate cells in validation spreadsheets “mt-atc-1\_2400d.xlsx” and “mt-atc-1\_9600d.xlsx” | Spreadsheets will update tables, graphics, and acceptance test results | | Copied concentrations from the output list file mt-atc-1.m3d for each time duration case and pasted into appropriate location in validation spreadsheets “mt-atc-1\_mt3d -sp-2400d.xlsx” (2400 days) and “mt-atc-1\_mt3d-sp-9600d.xlsx” (9600 days) for single precision executable tests, and “mt-atc-1\_mt3d -dp-2400d.xlsx” (2400 days) and “mt-atc-1\_mt3d-dp-9600d.xlsx” (9600 days) for double precision executable tests. Graphics updated with test results and acceptance test pass/fail conditions updated. Copies of these spreadsheets were maintained in appropriate testing subdirectories to allow for testing the single and double precision executable files separately. | |
| 6 | Use test results and graphics from spreadsheet to complete test reporting in ATR | Copy and paste graphics and note acceptance test results in ATR | MT3DMS acceptance test criterion are met | | Copy and pasted resulting graphics to the acceptance test report to show comparison of analytic and MT3DMS-MST results; noted results in ATR for acceptance criteria calculated in the spreadsheets “mt-atc-1\_mt3d-sp-2400d.xlsx” and “mt-atc-1\_mt3d-sp-9600d.xlsx” for single precision executable and spreadsheets “mt-atc-1\_mt3d-dp-2400d.xlsx” and “mt-atc-1\_mt3d-dp-9600d.xlsx” for double precision executable.  All criteria were met for this software.  Test directory contents were committed to MKS Integrity© for this test. | |

ATTACHMENT 6

Completed Test Log: MT3DMS Acceptance Test Case 1 (MT-ATC-1) for MT3DMS Executable Files for Linux® Operating System

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| MT3DMS Acceptance Test Case 1  Description: One-Dimensional Advective-Diffusive Transport | | | | Test Case #:  MT-ATC-1 | | Date:  3 Mar 2015 |
| System Attributes:  Version #: MT3DMS  Release #: CHPRC Build 8 (Identical to Build 7)  Environment: Redhat Enterprise Linux® release 5.8  Server: Tellus Linux® Cluster | | | | Test Performed by:  William E. Nichols, CHPRC  [Signed in Previous Revision 6 to this document] | | |
| Test Step # | Requirement # | Test Instruction | Expected Result | | Actual Result | |
| 1 | Obtain source code or executable for MODFLOW-2000-MST and MT3DMS code from software owner & install on target computer | Compile using appropriate Fortran compiler, if necessary | MODFLOW and MT3DMS executables are ready and functional | | Using installation of MODFLOW executable prepared and tested in previous acceptance test (MF-ATC-1).  Copied source code downloaded from MT3DMS maintenance site on 3-Feb-2015 and archived in MKS Integrity™ (2517) and placed in source directory on Tellus Linux® Cluster.  Developed “build-lahey-sp.sh” and “build-lahey-dp.sh”, to compile and link all necessary code to build the software executable files:   * Compiles all Fortran source code using Lahey Fortran Compiler for Linux® Release 8.01b compiler * Links all object files with required library statically   Code executable files are placed in executable test directory …/bin-test for testing and were named mf2k-chprc07spl.x and mf2k-chprc07dpl.x. | |
| 2 | Obtain files for test problem from software owner | Copy files to appropriate test directory | Test files are ready for use | | Files obtained from MKS Integrity™ for acceptance test case MT-ATC-1 copied entire test directory to …/test/modflow/build-7/mt3dms | |
| 3 | Run MODFLOW to solve for flow problem | Execute MODFLOW against mt-atc-1.nam name file in /flow test directory | MODFLOW executes without error; flow results transfer file is ready for use in next step | | Logged onto Tellus as a user that does not have administrator privileges. Confirmed that user’s “.bashrc” file set user in “test mode” with PATH variable pointing to executable files in test executable directory /bin-test rather than production directory /bin.  Executed MODFLOW against steady-state flow solution case without error; flow results prepared in transfer file mt-atc-1.ftl. | |
| 4 | Run MT3DMS to solve for transport in both time durations | Execute MT3DMS against mt-atc-1.nam name file in both /transport\_2400d and /transport\_9600d subdirectories | MT3DMS executes without error; transport results are available in mt-atc-1.m3d in both time solution subdirectories | | While logged onto Tellus as a user that does not have administrator privileges;  MT3DMS executed without error for both 2400 day and 9600 day transport duration cases for both single and double precision executable files. | |
| 5 | Extract results and transfer to validation spreadsheets | Using a text editor, copy MT3DMS-calculated concentration values from end of list file mf-atc-1.m3d and paste into appropriate cells in validation spreadsheets “mt-atc-1\_2400d.xlsx” and “mt-atc-1\_9600d.xlsx” | Spreadsheets will update tables, graphics, and acceptance test results | | Copied concentrations from the output list file mt-atc-1.m3d for each time duration case and pasted into appropriate location in validation spreadsheets “mt-atc-1\_mt3d -sp-2400d.xlsx” (2400 days) and “mt-atc-1\_mt3d-sp-9600d.xlsx” (9600 days) for single precision executable tests, and “mt-atc-1\_mt3d -dp-2400d.xlsx” (2400 days) and “mt-atc-1\_mt3d-dp-9600d.xlsx” (9600 days) for double precision executable tests. Graphics updated with test results and acceptance test pass/fail conditions updated. Copies of these spreadsheets were maintained in appropriate testing subdirectories to allow for testing the single and double precision executable files separately. | |
| 6 | Use test results and graphics from spreadsheet to complete test reporting in ATR | Copy and paste graphics and note acceptance test results in ATR | MT3DMS acceptance test criterion are met | | Copy and pasted resulting graphics to the acceptance test report to show comparison of analytic and MT3DMS-MST results; noted results in ATR for acceptance criteria calculated in the spreadsheets “mt-atc-1\_mt3d-sp-2400d.xlsx” and “mt-atc-1\_mt3d-sp-9600d.xlsx” for single precision executable and spreadsheets “mt-atc-1\_mt3d-dp-2400d.xlsx” and “mt-atc-1\_mt3d-dp-9600d.xlsx” for double precision executable.  All criteria were met for this software.  Test directory contents were committed to MKS Integrity© for this test. | |

ATTACHMENT 7

Completed Test Log: MT3DMS Acceptance Test Case 1 (MT-ATC-1): MT3DMS-MST Executable Files for Windows® Operating System

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| MT3DMS Acceptance Test Case 1  Description: One-Dimensional Advective-Diffusive Transport | | | | Test Case #:  MT-ATC-1 | | Date:  24 Nov 2015 |
| System Attributes:  Version #: MT3DMS-MST  Release #: CHPRC Build 8  Environment: Windows 7® Enterprise SP1  Server: WF22668 | | | | Test Performed by:  Joan Blainey, INTERA | | |
| Test Step # | Requirement # | Test Instruction | Expected Result | | Actual Result | |
| 1 | Obtain source code or executable for MODFLOW-2000-MST and MT3DMS code from software owner & install on target computer | Compile using appropriate Fortran compiler, if necessary | MODFLOW and MT3DMS executables are ready and functional | | For the flow solution used in this test, used the test installation of MODFLOW executable files mf2k-mst-chprc07spv.exe and mf2k-mst-chprc07dpv.exe that were prepared and tested in acceptance test (MF-ATC-1) noted in Attachment 2.  The source and executable code for MT3DMS obtained by FTP download in compressed archive form from SSP&A on 16-Nov-2015 was archived in MKS Integrity™ (2517). The provided executable files (MT3D\_Reaction\_dble.exe and MT3D\_Reaction\_sngl.exe) were renamed mt3d-mst-chprc08spl.exe (single precision) and mt3d-mst-chprc08dpl.exe (double precision) to denote CHPRC build 8 for testing.  Placed copies of these code executable files in directory c:\bin. | |
| 2 | Obtain files for test problem from software owner | Copy files to appropriate test directory | Test files are ready for use | | Files obtained from MKS Integrity™ for acceptance test case MT-ATC-1 were obtained and placed in test directory:  …\MODFLOW\_Build8\mt3dms-mst | |
| 3 | Run MODFLOW to solve for flow problem | Execute MODFLOW against mt-atc-1.nam name file in /flow test directory | MODFLOW executes without error; flow results transfer file is ready for use in next step | | Logged onto AUS-Gallium as a user without administrator privileges. Set the PATH variable pointed to executable files in test directory c:\bin\  Executed MODFLOW against steady-state flow solution case without error for single and double precision cases; flow results prepared in transfer file mt-atc-1.ftl. | |
| 4 | Run MT3DMS to solve for transport in both time durations | Execute MT3DMS against mt-atc-1.nam name file in both /transport\_2400d and /transport\_9600d subdirectories | MT3DMS executes without error; transport results are available in mt-atc-1.m3d in both time solution subdirectories | | MT3DMS executed without error for both 2400 day and 9600 day transport duration cases for both single and double precision executable files. | |
| 5 | Extract results and transfer to validation spreadsheets | Using a text editor, copy MT3DMS-calculated concentration values from end of list file mf-atc-1.m3d and paste into appropriate cells in validation spreadsheets “mt-atc-1\_2400d.xlsx” and “mt-atc-1\_9600d.xlsx” | Spreadsheets will update tables, graphics, and acceptance test results | | Copied concentrations from the output list file mt-atc-1.m3d for each time duration case and pasted into appropriate location in validation spreadsheets “mt-atc-1\_mt3d-mst-sp-2400d.xlsx” (2400 days) and “mt-atc-1\_mt3d-mst-sp-9600d.xlsx” (9600 days) for single precision executable tests, and “mt-atc-1\_mt3d-mst-dp-2400d.xlsx” (2400 days) and “mt-atc-1\_mt3d-mst-dp-9600d.xlsx” (9600 days) for double precision executable tests. Graphics updated with test results and acceptance test pass/fail conditions updated. Copies of these spreadsheets were maintained in appropriate testing subdirectories to allow for testing the single and double precision executable files separately. | |
| 6 | Use test results and graphics from spreadsheet to complete test reporting in ATR | Copy and paste graphics and note acceptance test results in ATR | MT3DMS acceptance test criterion are met | | Copy and pasted resulting graphics to the acceptance test report to show comparison of analytic and MT3DMS-MST results; noted results in ATR for acceptance criteria calculated in the spreadsheets “mt-atc-1\_mt3d-mst-sp-2400d.xlsx” and “mt-atc-1\_mt3d-mst-sp-9600d.xlsx” for single precision executable and spreadsheets “mt-atc-1\_mt3d-mst-dp-2400d.xlsx” and “mt-atc-1\_mt3d-mst-dp-9600d.xlsx” for double precision executable.  All criteria were met for this software.  Test directory contents were committed to MKS Integrity© for this test. | |

ATTACHMENT 8

Completed Test Log: MT3DMS Acceptance Test Case 1 (MT-ATC-1) for MT3DMS-MST Executable Files for Linux® Operating System

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| MT3DMS Acceptance Test Case 1  Description: One-Dimensional Advective-Diffusive Transport | | | | Test Case #:  MT-ATC-1 | | Date:  23 Nov 2015 |
| System Attributes:  Version #: MT3DMS-MST  Release #: CHPRC Build 8  Environment: Redhat Enterprise Linux® release 5.8  Server: Tellus Linux® Cluster | | | | Test Performed by:  Joan Blainey, INTERA | | |
| Test Step # | Requirement # | Test Instruction | Expected Result | | Actual Result | |
| 1 | Obtain source code or executable for MODFLOW-2000-MST and MT3DMS code from software owner & install on target computer | Compile using appropriate Fortran compiler, if necessary | MODFLOW and MT3DMS executables are ready and functional | | Using installation of MODFLOW executable prepared and tested in previous acceptance test (MF-ATC-1).  Copied source code downloaded from SSP&A FTP site in compressed archive form 16-Nov-2015 and archived in MKS Integrity™ (2517) and placed in source directory on INTERA’s Austin Linux® Cluster.  Developed scripts ‘build-ifort-sp.sh’ and ‘build-ifort-dp.sh’ to compile and link all necessary code to build two instances of the software executable, one single and one double precision. The build scripts:   * Compile Fortran source code using Intel Fortran (Version 13.0.1) for Linux® compiler * Link all object files with required library statically   Placed code executable files in CHPRC executable files directory …/test-Build8-linux and with file names mt3dms-mst-chprc08spl.x and mt3dms-mst-chprc08dpl.x for single and double precision compilations, respectively. | |
| 2 | Obtain files for test problem from software owner | Copy files to appropriate test directory | Test files are ready for use | | Files obtained from MKS Integrity™ for acceptance test case MT-ATC-1 copied entire test directory to  …/MODFLOW\_Build8/mt3dms-mst | |
| 3 | Run MODFLOW to solve for flow problem | Execute MODFLOW against mt-atc-1.nam name file in /flow test directory | MODFLOW executes without error; flow results transfer file is ready for use in next step | | Logged onto INTERA’s cluster as a user that does not have administrator privileges. Confirmed that executables in the build scripts point to executables in the test-Build8-linux directory.  Executed MODFLOW against steady-state flow solution case without error; flow results prepared in transfer file mt-atc-1.ftl. | |
| 4 | Run MT3DMS to solve for transport in both time durations | Execute MT3DMS against mt-atc-1.nam name file in both /transport\_2400d and /transport\_9600d subdirectories | MT3DMS executes without error; transport results are available in mt-atc-1.m3d in both time solution subdirectories | | While logged onto INTERA’s cluster as a user that does not have administrator privileges;  MT3DMS executed without error for both 2400 day and 9600 day transport duration cases for both single and double precision executable files. | |
| 5 | Extract results and transfer to validation spreadsheets | Using a text editor, copy MT3DMS-calculated concentration values from end of list file mf-atc-1.m3d and paste into appropriate cells in validation spreadsheets “mt-atc-1\_2400d.xlsx” and “mt-atc-1\_9600d.xlsx” | Spreadsheets will update tables, graphics, and acceptance test results | | Copied concentrations from the output list file mt-atc-1.m3d for each time duration case and pasted into appropriate location in validation spreadsheets “mt-atc-1\_mt3d-mst-sp-2400d.xlsx” (2400 days) and “mt-atc-1\_mt3d-mst-sp-9600d.xlsx” (9600 days) for single precision executable tests, and “mt-atc-1\_mt3d-mst-dp-2400d.xlsx” (2400 days) and “mt-atc-1\_mt3d-mst-dp-9600d.xlsx” (9600 days) for double precision executable tests. Graphics updated with test results and acceptance test pass/fail conditions updated. Copies of these spreadsheets were maintained in appropriate testing subdirectories to allow for testing the single and double precision executable files separately. | |
| 6 | Use test results and graphics from spreadsheet to complete test reporting in ATR | Copy and paste graphics and note acceptance test results in ATR | MT3DMS acceptance test criterion are met | | Copy and pasted resulting graphics to the acceptance test report to show comparison of analytic and MT3DMS-MST results; noted results in ATR for acceptance criteria calculated in the spreadsheets “mt-atc-1\_mt3d-mst-sp-2400d.xlsx” and “mt-atc-1\_mt3d-mst-sp-9600d.xlsx” for single precision executable and spreadsheets “mt-atc-1\_mt3d-mst-dp-2400d.xlsx” and “mt-atc-1\_mt3d-mst-dp-9600d.xlsx” for double precision executable.  All criteria were met for this software.  Test directory contents were committed to MKS Integrity© for this test. | |

ATTACHMENT 9

Completed Test Log: MODFLOW Acceptance Test Case 1 (MF-ATC-1): MODFLOW-USG Executable Files for Windows® Operating System

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| MODFLOW Acceptance Test Case 1  Description: Theis Transient Drawdown Problem | | | Test Case #:  MF-ATC-1 | Date:  8 May 2015 |
| System Attributes:  Version #: MODFLOW-USG  Release #: CHPRC Build 8 (Identical to Build 7)  Environment: Windows 8.1 Pro | | | Test Performed by:  Joan B. Blainey, INTERA  [Signed in Previous Revision 7 to this document] | |
| Test Step # | Requirement # | Test Instruction | Expected Result | Actual Result |
| 1 | Obtain source code or executable for MODFLOW-USG code from software owner & install on target computer | Compile using appropriate Fortran compiler, if necessary | MODFLOW executable is ready and functional | Source code and Windows® executable files obtain by download from USGS site on 29-Apr-2015. Executable was copied from […/MODFLOW-USG-acceptance-test](file:///\\psc-amber\DFS\Projects\PSC\wnichols\MODFLOW-USG-acceptance-test) to target computer and placed in …/bin |
| 2 | Obtain files for test problem from software owner | Copy files to appropriate test directory | Test files are ready for use | Files obtained from […\MODFLOW-USG-acceptance-test](file:///\\psc-amber\DFS\Projects\PSC\wnichols\MODFLOW-USG-acceptance-test) were copied to directory …\bin |
| 3 | Run MODFLOW to solve for flow problem | Execute MODFLOW against mf-atc-1.nam name file in test directory | MODFLOW executes without error | Logged onto machine with a user account that does not have administrator privileges.  Successfully executed mfusg-chprc07spl.exe and mfusg-chprc07dpl.exe for both pumping duration (in subdirectories /pumping-05-d and /pumping-10-d) by running the batch file “run-install-tests.bat” for the *χ*MD solver and the batch file “run-install-tests\_pcgu.bat” for the PCGU solver. |
| 4 | Extract results and transfer to validation spreadsheet | Using a text editor, copy MODFLOW-calculated drawdown values from end of list file mf-atc-1.lis and paste into appropriate cells in validation spreadsheet “mt-atc-1.xlsx” | Spreadsheet will update tables, graphics, and acceptance test results | Used a text editor program to open the theis.lst file for each pumping duration case with the *χ*MD solver and copied the drawdown for the first row of results that represent the radial drawdown results. Pasted these results into the respective copies of the Excel® validation spreadsheets “mf-atc-1\_mst-sp.xlsx” for single precision results and “mf-atc-1\_mfusg-dp.xlsx” for double precision results.  A similar process was conducted for the PCGU solver. Used a text editor program to open the theis.lst file for each pumping duration case with the PCGU solver and copied the drawdown for the first row of results that represent the radial drawdown results. Pasted these results into the respective copies of the Excel® validation spreadsheets “mf-atc-1\_mst-sp\_pcgu.xlsx” for single precision results and “mf-atc-1\_mfusg-dp\_pcgu.xlsx” for double precision results. |
| 5 | Use test results and graphics from spreadsheet to complete test reporting in ATR | Copy and paste graphics and note acceptance test results in ATR | MODFLOW acceptance test criterion are met | Copy and pasted resulting graphics to the acceptance test reports to show comparison of analytic and MODFLOW results; noted results in ATR for acceptance criteria calculated in copies the spreadsheets “mf-atc-1\_mfusg-sp.xlsx” and “mf-atc-1\_mfusg-dp.xlsx” for each repeated test by precision for the *x*MD solver.  All criteria were met for this software using the *x*MD solver.  Copy and pasted resulting graphics to the acceptance test reports to show comparison of analytic and MODFLOW results; noted results in ATR for acceptance criteria calculated in copies the spreadsheets “mf-atc-1\_mfusg-sp\_pcgu.xlsx” and “mf-atc-1\_mfusg-dp\_pcgu.xlsx” for each repeated test by precision for the PCGU solver.  Not all the test criteria were met for this software using the PCGU solver.  Test directory contents were committed to MKS Integrity© for this test. |

ATTACHMENT 10

Completed Test Log: MODFLOW Acceptance Test Case 1 (MF-ATC-1): MODFLOW-USG Executable Files for Linux® Operating System

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| MODFLOW Acceptance Test Case 1  Description: Theis Transient Drawdown Problem | | | Test Case #:  MF-ATC-1 | Date:  1 May 2015 |
| System Attributes:  Version #: MODFLOW-USG  Release #: CHPRC Build 8 (Identical to Build 7)  Environment:: OS: GNU/Linux®; Kernel: Linux®;  Distribution: Kernel version 2.6.32-358.11.1.el6.centos.plus.x86\_64  Server: INTERA’s Austin Linux® Cluster | | | Test Performed by:  Joan B. Blainey, INTERA  [Signed in Previous Revision 7 to this document] | |
| Test Step # | Requirement # | Test Instruction | Expected Result | Actual Result |
| 1 | Obtain source code or executable for MODFLOW-USG code from software owner & install on target computer | Compile using appropriate Fortran compiler, if necessary | MODFLOW executable is ready and functional | Source code obtain by download from USGS site on 29-Apr-2015. Executable was copied from […\MODFLOW-USG-acceptance-test](file:///\\psc-amber\DFS\Projects\PSC\wnichols\MODFLOW-USG-acceptance-test) to target computer and placed in \*\*\* directory on INTERA’s Linux® cluster located in the Austin office.  Developed “makefile” and makefile\_dp”, for the single and double precision executables, respectively. Executed the commands “make -f makefile” and “make-f makefile\_dp” to compile, link, and create the software executable files:   * Compiles are Fortran source code using the Intel Fortran Compiler for Linux® version 13.0.1 * Links all object files with required libraries statically.   Executables files were placed in the test directory at …/test/ and are named mfusg-chprc07spl.x and mfusg-chprc07dpl.x for the single and double precision executable files, respectively. |
| 2 | Obtain files for test problem from software owner | Copy files to appropriate test directory | Test files are ready for use | Copied acceptance test case files from […\MODFLOW-USG-acceptance-test](file:///\\psc-amber\DFS\Projects\PSC\wnichols\MODFLOW-USG-acceptance-test) to directory …/test-linux/mfusg in appropriate directories for separately testing the single and double precision executable files. |
| 3 | Run MODFLOW to solve for flow problem | Execute MODFLOW against mf-atc-1.nam name file in test directory | MODFLOW executes without error | Logged onto INTERA’s linux cluster in Austin with the jblainey user account which does not have administrator privileges.  Created a shell script “run-install-test-one-node\_jbb.sh” that successfully executes in both pumping duration subdirectories for both the single precision and double precision executables for the . These subdirectories are:   * …/test-linux/mfusg/mf-atc-1/sp/pumping-05-d * …/test-linux/mfusg/mf-atc-1/sp/pumping-10-d * …/test-linux/mfusg/mf-atc-1/dp/pumping-05-d * …/test-linux/mfusg/mf-atc-1/dp/pumping-10-d   Each of the runs was configured with the *x*MD solver. |
| 4 | Extract results and transfer to validation spreadsheet | Using a text editor, copy MODFLOW-calculated drawdown values from end of list file mf-atc-1.lis and paste into appropriate cells in validation spreadsheet “mt-atc-1.xlsx” | Spreadsheet will update tables, graphics, and acceptance test results | Used the text editor program vi to open the theis.lst file for each pumping duration case and copied the drawdown for the first row of results, representing the radial drawdowns. Pasted these results into the respective copies of the worksheets “mf-atc-1\_mfusg-sp.xlxs” and “mf-atc-1\_mfusg-dp.xlsx”. |
| 5 | Use test results and graphics from spreadsheet to complete test reporting in ATR | Copy and paste graphics and note acceptance test results in ATR | MODFLOW acceptance test criterion are met | Copy and pasted resulting graphics to the acceptance test reports to show comparison of analytic and MODFLOW results; noted results in ATR for acceptance criteria calculated in copies the spreadsheets “mf-atc-1\_mfusg-sp.xlsx” and “mf-atc-1\_mfusg-dp.xlsx” for each repeated test by precision for the xMD solver.  All criteria were met for this software using the xMD solver.  Test directory contents were committed to MKS Integrity© for this test. |

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