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README FILE FOR MT3DMS 4.5  
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Chunmiao Zheng ([czheng@ua.edu](mailto:czheng@ua.edu))  
University of Alabama  
Last revision: 05-28-2003

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GENERAL INFORMATION  
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MT3DMS is a 3-D multispecies contaminant fate and transport model developed at the University of Alabama for the US Army Corps of Engineers Research and Development Center. Detailed information on MT3DMS can be found in MT3DMS Documentation and User's Guide (Zheng and Wang, 1999), available at <http://hydro.geo.ua.edu/mt3d>.

Additional information specific to MT3DMS since version 4.0 can be found in U.S. Geological Survey Open-File Report 01-82 by Zheng, Hill and Hsieh (2001), also available at <http://hydro.geo.ua.edu/mt3d>.

To report any program errors, please contact

Chunmiao Zheng  
Department of Geological Sciences  
University of Alabama  
202 Bevill Building  
Tuscaloosa, AL 35487, USA  
Phone: (205) 348-0579  
E-mail: [czheng@ua.edu](mailto:czheng@ua.edu)  
<http://hydro.geo.ua.edu/mt3d>

EXECUTABLE PROGRAMS AND SYSTEM REQUIREMENTS  
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Two MT3DMS executables, **mt3dms4s.exe** and **mt3dms4b.exe**, are included with the distribution files (the differences between the two are explained in the next section). The executable programs were compiled with Lahey

FORTRAN 95 compiler (LF95) Version 5.7 to run on PCs with Pentium or higher CPUs. MT3DMS allows dynamic memory allocation and will allocate the exact amount of memory that is required for a particular problem at run-time. If the memory required by the problem exceeds the total amount of physical memory (RAM) that is available, MT3DMS will automatically use hard-drive space as virtual memory. However, this slows down computations dramatically. Thus, it is best to have sufficient RAM to run any particular model. MT3DMS runs under any recent version of Microsoft Windows in a command-prompt window.

#### NOTES ON THE UNFORMATTED FLOW-TRANSPORT LINK FILE

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The interface between MODFLOW and MT3DMS is through a flow-transport link file saved by the Link-MT3DMS (LMT) Package added to MODFLOW. The flow-transport link file is usually saved as unformatted (binary characters). (An option available in the LMT6 Package for MODFLOW-2000 allows the link file to be saved as an ascii text file, but the file size may be so large that the option is generally limited to small models.) Different FORTRAN compilers or even different versions of the same compiler may use different file structures and styles for the unformatted binary files. For this reason, the MT3DMS code compiled by a particular compiler may not be able to read the unformatted flow-transport link file saved by a MODFLOW code that was compiled with a different compiler, and vice versa.

Two versions of MT3DMS executable are included with the distribution files. Both versions were compiled using Lahey Fortran 95 compiler (LF95). The only difference between the two versions is in the style of unformatted files as specified in the source include file 'filespec.inc'.

The standard version, **mt3dms4s.exe**, was compiled with standard Fortran file specifiers for the unformatted files, i.e.,

**FORM='unformatted' and ACCESS='sequential'**

The resulting unformatted files are compatible with those of Visual Fortran from HP/Compaq. However, they are not compatible with those of earlier Lahey compilers including LF77 and LF90. Thus, an existing flow-transport link file generated by a MODFLOW code compiled by LF77 and LF90 needs to be regenerated for use by **mt3dms4s.exe**. A utility program, LF90to95.exe, could also be used to convert the LF77/LF90-styled unformatted file to the LF95-styled. Since MODFLOW-96 and MODFLOW-88 included with the MT3DMS distribution files were also compiled with the same standard file specifiers, the version of MT3DMS executable for use with MODFLOW-96 and MODFLOW-88 should be **mt3dms4s.exe**.

The other executable, **mt3dms4b.exe**, was compiled with the following file specifiers for the unformatted files:

**FORM='binary' and ACCESS='sequential'**

where FORM='binary' is a non-standard Fortran feature that may or may not be available to a specific compiler. The resulting unformatted files are also referred to as unstructured, true binary files. An unstructured, true binary file is not compiler specific, thus, it makes it possible for the resulting MT3DMS code to read unformatted files that are generated by non-Lahey compilers, as long as they are also of the unstructured, true binary nature. The same non-standard file specifier has been used for MODFLOW-2000 since version 1.2. Thus, the version of MT3DMS executable for use with MODFLOW-2000 should be **mt3dms4b.exe**.

## INSTALLATION AND RE-COMPILING

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The distribution file is a self-extracting program. Execution of the distribution file creates numerous individual files. The extraction program allows you to specify the directory in which the files should be restored. The installation instructions assume that the files are restored into directory C:\MT3DMS4. The following directory structure will be created in C:\MT3DMS4:

```
|
|--MT3DMS4
|   |--bin      ; compiled executables
|   |--doc      ; documentation files
|   |--src      ; source code
|   |--examples ; benchmark test problems
|   |--utility  ; utility programs
```

To make the executable programs in "\MT3DMS4\bin" accessible from any directory, the path of the subdirectory "\MT3DMS4\bin" should be included in the PATH environment variable. For example, you could add a line similar to the following to the AUTOEXEC.BAT file:

```
PATH=%PATH%;C:\MT3DMS4\bin
```

Make sure to substitute the appropriate drive letter and pathname if not C:\ as shown above. Reboot your system after modifying AUTOEXEC.BAT.

On Windows 2000/NT/XP systems, from the Start menu, find and select Control Panel. Then edit the PATH Environment Variable to include "C:\MT3DMS4\bin". Initiate and use a new MS-DOS Command Prompt window after making this change.

To re-compile this version MT3DMS with Lahey LF95, copy all source files to a temporary subdirectory and type 'AM' to start the AUTOMAKE utility. The compiler options that should be used for recompiling are contained in the file Automake.fig. MT3DMS was written in standard ANSI FORTRAN 77 plus some elements of FORTRAN 90, and can be compiled by most FORTRAN 77, 90 or 95 compilers with little or no modification.

## RUNNING THE SOFTWARE

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To run MT3DMS 4.5 using the Name-File method, enter the command

```
mt3dms4s [name-file]
```

where the command-line argument [name-file] is the name of the MT3DMS name-file as described in Zheng, Hill and Hsieh (2001). If no command-line argument is given, the user is prompted to enter the name of the name-file. If the file name ends with the extension ".nam", it can be specified without including the extension. For example, if the name-file is named "project.nam", the simulation can be run by entering:

```
mt3dms4s project
```

If the user hits the Enter key when prompted to enter the name of the name-file, MT3DMS will proceed to prompt the user for the various input/output file names, as in all versions prior to 4.0. It is still possible to put all these file names in a response file and run MT3DMS 4.5 by entering

```
mt3dms4s < response.fil
```

where response.fil is the name of the response file. Note that the first line of the response file needs to be left blank.

## INTERFACE WITH MODFLOW-96 AND MODFLOW-88

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A version of the standard USGS MODFLOW-96 code implemented with the Link-MT3D Package v5 is included with the MT3DMS distribution files. This version of MODFLOW-96 is named mf96.exe. To activate the LMT Package to save the flow-transport file needed by MT3DMS, insert a line (shown in capital letters) into the MODFLOW-96 NAME file as in the following example:

An example of MODFLOW-96 NAME file:

```
list 6 test1.lst
bas 1 test1.bas
bcf 11 test1.bcf
sip 13 test1.sip
oc 14 test1.oc
LMT 32 TEST1.FTL
data(binary) 93 test1.ufh
```

where LMT is the name of the Link-MT3D package, integer 32 is the FORTRAN unit on which the MODFLOW-MT3D link file will be saved, and TEST1.FTL is the name of the MODFLOW-MT3D link file containing the flow model information needed by MT3DMS. The unit for LMT can be any

positive integer as long as it has not been used for any other files. Any valid file name can be specified by the user for the MODFLOW-MT3D link file. When running MT3DMS, make sure to enter the same file name, e.g., TEST1.FTL in this example.

More information on using MODFLOW-96 with MT3DMS can be found in the document README\_MF96LMT.pdf. The source code for MODFLOW-96 with the Link-MT3D interface can be downloaded from <http://hydro.geo.ua.edu/mt3d>.

A version of the standard USGS MODFLOW-88 code implemented with the Link-MT3D Package v3 is also included with the MT3DMS distribution files. This version of MODFLOW-88 is named mf88.exe. For more information on using MODFLOW-88 with MT3DMS, refer to the document README\_MF88LMT.pdf. The source code for MODFLOW-88 with the Link-MT3D interface can also be downloaded from <http://hydro.geo.ua.edu/mt3d>.

#### INTERFACE WITH MODFLOW-2000

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The linkage between MT3DMS and MODFLOW-2000 is through the Link-MT3DMS (LMT6) Package (LMT6) added to MODFLOW-2000 since version 1.4. The input file for the LMT6 Package is associated with the file type "LMT6". To activate the LMT6 Package in MODFLOW-2000, the user needs to insert a line as shown below into the Name file of MODFLOW-2000:

```
#
# Link-MT3DMS input file
lmt6      66      test1.lmt
#
```

where "test1.lmt" is the name of the input file for the LMT6 Package which specifies the name of the flow-transport link file and how it should be saved by MODFLOW-2000 for use by MT3DMS. It is noteworthy that, with MODFLOW-96, the name of the flow-transport link file is directly specified in the NAME file of MODFLOW-96 following the "**LMT**" keyword, while with MODFLOW-2000, the name of flow-transport link file is specified in an input file to the LMT6 Package. It is the name of the LMT6 input file that follows the keyword "**LMT6**". The details of the MODFLOW-2000 and MT3DMS linkage and the input instructions for the LMT6 Package input file are provided in Zheng, Hill and Hsieh (2001).

#### LIST OF FILES

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Readme_MT3DMS.txt:	latest readme file (this file)
Readme_MT3DMS.pdf:	latest readme file in PDF format
upgrade.pdf:	bug fixes, enhancements, and version history
upgrade.htm:	upgrade.txt in HTML format

### **Subdirectory \bin**

mt3dms4s.exe: MT3DMS executable (for use with standard unformatted flow-transport link files)  
mt3dms4b.exe: MT3DMS executable (for use with unstructured true-binary flow-transport link files)  
mf2k.exe: modflow-2000 executable (v. 1.11)  
mf96.exe: modflow-96 executable  
mf88.exe: modflow-88 executable  
pm.exe: PostMT3DMS utility  
savelast.exe: SaveLast utility  
LF90to95.exe: LF90-style to LF95-style unformatted file converter  
LF95to90.exe: LF95-style to LF90-style unformatted file converter  
Bin2Unf.exe: True-binary to LF95-style unformatted file converter  
Unf2Bin.exe: LF95-style to true-binary unformatted file converter

### **Subdirectory \doc**

MT3DMS\_manual.pdf: MT3DMS User's Manual (Zheng and Wang, 1999)  
OFR01-82(LMT6).pdf: User's Guide for Link-MT3DMS (LMT6) Package for MODFLOW-200  
Readme\_MF96LMT.pdf: Readme file for MODFLOW-96 with Link-MT3D interface 5.0  
Readme\_MF88LMT.pdf: Readme file for MODFLOW-88 with Link-MT3D interface 3.0  
Readme\_Uutilities.pdf: Readme file for MT3DMS utilities

### **Subdirectory \src**

mt3dms4.for: source file for MT3DMS main program  
mt\_btn4.for: source file for MT3DMS Basic Transport package  
mt\_adv4.for: source file for MT3DMS Advection package  
mt\_dsp4.for: source file for MT3DMS Dispersion package  
mt\_ssm4.for: source file for MT3DMS Sink & Source Mixing package  
mt\_rct4.for: source file for MT3DMS Chemical Reaction package  
mt\_gcg4.for: source file for MT3DMS GCG Solver package  
mt\_fmi4.for: source file for MT3DMS Flow Model Interface package  
mt\_utl4.for: source file for MT3DMS Utility package  
filespec.inc: 'include' file with file specifiers  
automake.fig: LF95 compiler options

### **Subdirectory \examples**

p~~x~~mt.nam: MT3DMS Name file for benchmark test problem no. x.  
p~~x~~mf.nam: MODFLOW Name file for benchmark test problem no. x.

### **Subdirectory \utility**

pm.for: source file for PostMT3DMS utility  
savelast.for: source file for SaveLast utility