MT3DMS v5.2
Supplemental User's Guide

Chunmiao Zheng
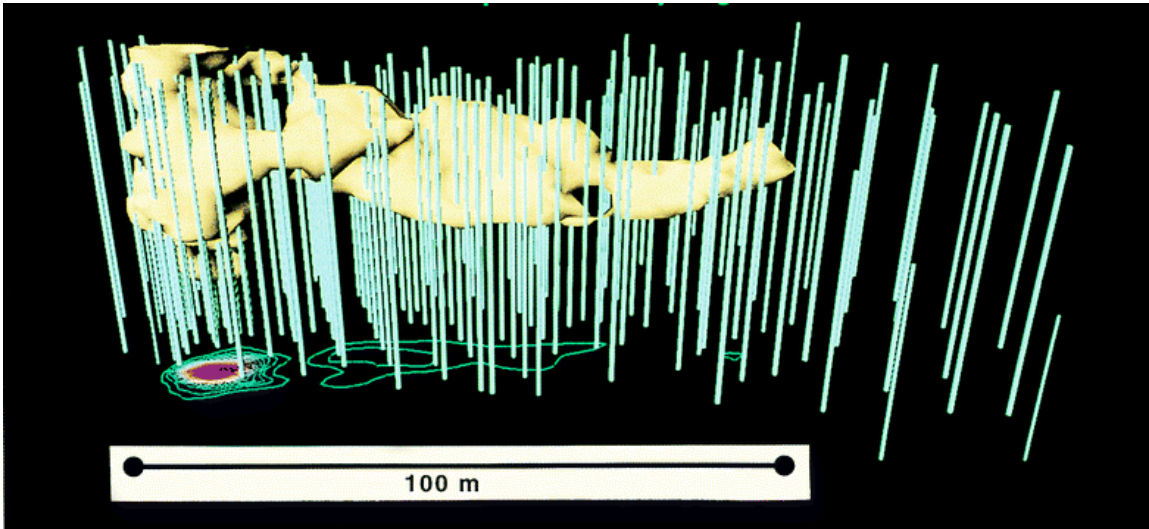
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MT3DMS v5.2

a modular three-dimensional multispecies transport model
for simulation of advection, dispersion and chemical reactions
of contaminants in groundwater systems

Supplemental User's Guide

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This program and the latest updates can be downloaded
from the MT3D home page at:

http://hydro.geo.ua.edu/mt3d

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Cover image from the work published by
Charles Harvey and Steve Gorelick.
Shown on the cover image is the bromide plume
measured at the MADE tracer experiment site
inside the Columbus Air Force Base
in Columbus, Mississippi.

Preface

This document describes the cumulative changes and enhancements made since Version 5.0 of the MT3DMS solute fate and transport model. It is intended as a supplement to the original MT3DMS Documentation and User's Guide published by the U.S. Army Corps of Engineers (Zheng and Wang, 1999; available at http://hydro.geo.ua.edu/mt3d). Readers should refer to Zheng and Wang (1999) for complete information on the theoretical background, numerical implementation, input instructions, and application examples for the MT3DMS model.

Table of Contents

1   Introduction

This document describes the cumulative changes and enhancements made since Version 5.0 of the MT3DMS solute fate and transport model and discusses all the new features that have become available since Version 5.0. It is intended as a supplement to the original MT3DMS Documentation and User's Guide (Zheng and Wang, 1999). For the most up-to-date information on MT3DMS, refer to the README file included with the distribution files.

There are a couple of significant organizational changes to Version 5 compared to the previous Version 4. First, the Name-File procedure becomes the only method to start a MT3DMS simulation run since v5.0. A Name-File specifies the names of most input and output files used in a model simulation. In addition, it controls the parts of the model program that are active, i.e., the "packages" that are used in the current simulation. Second, the implicit matrix solver, the General Conjugate-Gradient (GCG) solver, must be used in every simulation since v5.0. In other words, the dispersion, sink/source and reaction terms are now always solved by the implicit finite-difference method, regardless of whether the advection term is solved by the implicit finite-difference method, the mixed Eulerian-Lagrangian methods, or the third-order TVD method.

A major new feature for MT3DMS since v5.0 is the Transport Observation (TOB) Package to save the calculated concentration at any observation location within the model domain and the calculated mass flux at any sink/source location. The calculated values are saved to output files, and optionally, along with the statistics of residuals between the calculated and observed values at the observation locations. The calculated concentrations can be interpolated from the nodal values if the observation point does not coincide with a model node. The calculated mass flux can be defined over any arbitrary group of sink/source cells referred to as a mass flux object.

Another important addition to MT3DMS since v5.0 is the support for the Multi-Node Well (MNW) Package (Halford and Hanson, 2002) used by MODFLOW-2000 (Harbaugh et al., 2000) to simulate the flow to a well screened over multiple nodes (layers). The MNW Package automatically partitions the total flow prescribed for a MNW into individual nodes (layers) and determines a single head value in the wellbore. Accordingly, MT3DMS computes a single composite concentration for the same wellbore based on the flux-weighted concentrations of the injected fluid (if any) and the flow rates from different layers.

Since Version 5.0, MT3DMS has also added support for more new MODFLOW sink/source packages, including Drain with Return Flow (DRT) and Evapotranspiration with a Segmented Function (ETS), both documented in Banta (2000). The DRT Package in MODFLOW-2000 simulates the re-injection of a portion of the outflow from a drain cell back into the aquifer. MT3DMS assigns the concentration at the outflow cell as that

of the re-injected source at the return drain-flow location. The ETS package is supported in a manner similar to the original EVT package.

New since Version 5.1 is the capability to simulate zeroth-order reactions in both single- and dual-domain systems. The standard MT3DMS code prior to v5.1 includes only the first-order kinetic reactions in the Chemical Reaction (RCT) Package. However, zeroth-order reactions may be useful for describing certain types of biogeochemical decay or production. In addition, zeroth-order reactions are needed in direct simulation of groundwater ages (e.g., Goode, 1996) and calculation of parameter sensitivities (e.g., Tsai et al., 2003). Thus starting with Version 5.1, zeroth-order reactions are available as a standard option through the RCT Package in either single- or dual-domain formulation.

Version 5.2 introduces a new option to include multicomponent and/or three-dimensional diffusion coefficients in the transport simulation. Prior to v5.2, the molecular diffusion coefficient can only be specified on a layer-by-layer basis (i.e., one uniform diffusion coefficient per model layer). Moreover, all solute components are assumed to have the same diffusion coefficient. Starting with Version 5.2, users are permitted to specify different diffusion coefficients for different solute components on a cell-by-cell basis (i.e., one diffusion coefficient per model cell, if necessary).

Another new feature since Version 5.2 is the capability to simulate a "recirculation well." A recirculation well refers to an injection well whose input concentration is not user-specified, but set internally equal to that of extracted water from a pumping well. This option is convenient for modeling some commonly encountered field situations, such as a "dipole" tracer test.

2. Running MT3DMS Using the Name-File Method

2.1 BACKGROUND

Starting with version 5.0, the only method to start a MT3DMS simulation is through a Name File that is similar to the Name File used by MODFLOW-96 and MODFLOW-2000. The Name-File method has been available in MT3DMS since version 4 as an optional method of starting a transport simulation (see Zheng et al., 2001). However, it has become the only method to initiate a transport run since MT3DMS v5.0. As a result, the Transport Option (TRNOP) array specified through the Basic Transport (BTN) Package of MT3DMS v5.1 no longer has any effect. However, the input line must still be specified in the BTN input file for backward compatibility reasons.

2.2 INPUT INSTRUCTIONS

The Name File contains the names of most input and output files used in a model simulation and controls the parts of the model program that are active. The Name File is read on unit 99, which is specified in the MT3DMS main program. The Name File is constructed as follows:

FOR EACH SIMULATION

1. Ftype   Nunit   Fname   [options]

The Name File contains one of the above records (item 1) for each file. All variables are free format. The length of each record must be 199 characters or less. The records can be in any order except for the record where Ftype (file type) is 'LIST' as described below.

Comment records are indicated by the # character in column 1 and can be located anywhere in the file. Any text characters can follow the # character. Comment records have no effect on the simulation; their purpose is to allow users to provide documentation about a particular simulation. All comment records after the first item-1 record are written in the listing file.

Explanation of Variables in the Name File

Ftype - is the file type, which must be one of the following character values. Ftype may be entered in all uppercase, all lowercase, or any combination.

LIST for the standard MT3DMS output file – the Name File for MT3DMS must always include a record that specifies 'LIST' for Ftype and the LIST record must be the first non-comment record.

BTN for the MT3DMS Basic Transport Package.
FTL for the MODFLOW-produced flow-transport link file.
ADV for the MT3DMS Advection Package.
DSP for the MT3DMS Dispersion Package.
SSM for the MT3DMS Sink/Source Mixing Package.
RCT for the MT3DMS Reaction Package.
GCG for the MT3DMS Generalized Conjugate-Gradient Solver Package.
TOB for the MT3DMS Transport Observation Package.

DATA(BINARY) for binary (unformatted) files such as those used for input of concentrations saved in a previous simulation as the initial condition for a continuation run.

DATA for formatted (text) files such as those used to save formatted concentrations at observation points and mass budget summaries or for input of data from files that are separate from the primary package input files.

Various output control options of MT3DMS can be set up to save several optional output files: the unformatted (binary) concentration file, the formatted concentration observation file, the formatted mass budget summary file, and the model configuration file. MT3DMS always assigns default names to these files with the conventions listed below. These default names can be overridden, as explained in the next paragraph.
- **MT3Dnnn.UCN** for the dissolved-phase unformatted concentration files where **nnn** is the species index number such as 001 for species 1, 002 for species 2, and so on;
- **MT3DnnnS.UCN** for the sorbed-phase or immobile-liquid-phase unformatted concentration files where **nnn** is the species index number such as 001 for species 1, 002 for species 2, and so on;
- **MT3Dnnn.OBS** for the formatted concentration observation files;
- **MT3Dnnn.MAS** for the formatted mass budget summary files; and
- **MT3D.CNF** for storing the model configuration (spatial discretization) information needed by post-processing programs. It is always saved along with the UCN files.

Nunit - is the FORTRAN unit to be used when reading from or writing to the file. Any valid unit number on the computer being used can be specified except for the unit numbers that have been internally preserved by the MT3DMS program, as listed in Table 2.1. To use the preserved unit number for a particular file, simply set Nunit associated with that file to 0. If a preserved unit is used for a file for which the unit is not intended, an error may occur and the program execution will be terminated. To avoid potential

errors, avoid using any units between 1 and 20, and any units above 100, when specifying units for those files that do not have a preserved unit (i.e., not listed in Table 2.1).

As pointed out previously, MT3DMS assigns the default file names for 'UCN', 'OBS', 'MAS' and 'CNF' files as MT3Dnnn.UCN, MT3DnnnS.UCN, MT3Dnnn.OBS, MT3Dnnn.MAS, and MT3D.CNF. To keep the results from a previous simulation, these files need to be renamed before starting a new simulation in the same directory. Otherwise, they will be overwritten by the files from the new simulation. It is possible to override these default names. To specify a different name for an unformatted 'UCN' file, for example, add a line as shown below into the MT3DMS Name File:

```
DATA(BINARY)   Nunit   NewRun.UCN
```

where Nunit must be a preserved unit for a particular species. For example, if the NewRun.UCN is intended for saving the unformatted concentration of species 1, then Nunit must be set to 201, i.e., the unit preserved for species 1 (see Table 2.1). Similarly, if the NewRun.UCN is intended for species 2, then Nunit must be set to 202.

To specify a different name for the formatted 'OBS', 'MAS' and 'CNF' files, insert a line as shown below into the MT3DMS Name File

```
DATA   Nunit   NewRun.OBS
```

where again Nunit must be a preserved unit for a particular species. For example, if NewRun.OBS is intended for saving the species 1 concentrations at the observation points, then Nunit must be set to 401, the unit preserved for species 1 (see Table 2.1). Similarly, if the NewRun.OBS is intended for species 2, then Nunit must be set to 402.

Fname - is the name of the input/output file, which is a character value. Pathnames may be specified as part of Fname.

[Options] – optional keywords that may be used for the corresponding input/output file. Currently, only two such keywords, FREE and PRINT, may be specified in conjunction with the flow-transport link (FTL) file. If the keyword FREE is specified, it indicates that the FTL input file for MT3DMS is in list-directed (free) format, i.e., produced by the LMT6 Package with the option OUTPUT_FILE_FORMAT set to formatted. If the keyword PRINT is specified, the content of the flow-transport link file is printed to the standard output file for checking and debugging purposes. Note that if no keyword is specified after the FTL file name, the FTL file is assumed to be unformatted (binary) by default.

Table 2.1. Preserved unit numbers for various file types in MT3DMS.

MT3DMS Input/Output Files	File Type	Preserved Unit
Output Listing File*	LIST	16
Package Options		
Basic Transport*	BTN	1
Flow-Transport Link*	FTL	10
Advection	ADV	2
Dispersion	DSP	3
Sink/Source Mixing	SSM	4
Reaction	RCT	8
Generalized Conjugate Gradient	GCG	9
Transport Observation	TOB	7
Output Files		
Model Configuration File	CNF	17
Unformatted Concentration File (dissolved phase)	UCN	200+species index
Unformatted Concentration File (sorbed/immobile phase)	UCN	300+species index
Concentrations Observation File	OBS	400+species index
Mass Budget Summary File	MAS	600+species index

*Note: these files are always required for every simulation.

An example of the MT3DMS Name File is shown below:

```
#
# MT3DMS Name File for a test problem
#
# Standard output
list      0  test1.m3d
#
# Input files
btn       0  test1.btn
adv       0  test1.adv
dsp       0  test1.dsp
ssm       0  test1.ssm
rct       0  test1.rct
gcg       0  test1.gcg
ftl       0  test1.ftl
```

In the example above, the FTL file 'test1.ftl' is treated as an unformatted (binary) file by default. If 'test1.ftl' is an ascii text file in free format, the last line should be modified as

```
ftl        0  test1.ftl     Free
```

Moreover, if the option print is specified as follows,

```
ftl        0  test1.ftl     print
```

Then the contents of the flow-transport link file read by MT3DMS will be echoed in the standard text output file generated by MT3DMS.

Further note that in the example above, no names are given for the unformatted concentration, formatted concentration observation, mass budget summary, and model configuration files. As a result, these files will be named, by default, MT3D001.UCN, MT3D001S.UCN, MT3D001.OBS, MT3D001.MAS, MT3D.CNF. To associate these files with different names, the Name File shown above can be modified by adding the following lines:

```
data(binary)  201  test1.ucn
data(binary)  301  test1s.ucn
data          401  test1.obs
data          601  test1.mas
data          17   test1.cnf
```


2.3 PROGRAM EXECUTION

To use the Name File method to start an MT3DMS simulation, the Name File must be created first. The name of the Name File can then be passed to MT3DMS through the command line argument as follows:

C:\MT3DMS5\Bin\MT3DMS5x Name-File

where **MT3DMS5x** is the name of the MT3DMS v5 executable program (where **x** denotes either **s** for the executable program using the standard unformatted files; and **b** for the executable program using the true binary files), and **Name-File** is the name of the MT3DMS Name File for a particular simulation. If no command line argument is specified, the user will be prompted to provide the name of the Name File interactively from the keyboard. The name of a Name File is assumed to have the 3-letter extension ".nam" by default if no extension is given when the Name File is specified from the command-line or interactively.

3 Using the New Transport Observation Package

3.1 BACKGROUND

In previous versions of MT3DMS, the user can specify the layer, row and column indices of any model nodes of interest where the calculated concentration values will be saved to one or more optional concentration observation (OBS) output files. If the user needs to obtain the calculated concentration at an observation point that does not coincide with a model nodal point, neighboring nodal concentrations must be saved and an interpolation performed outside the MT3DMS code. This can be quite cumbersome. Moreover, there is no capability in previous versions to save the calculated mass fluxes at any sink/source locations.

A new Transport Observation (abbreviated as "TOB") Package has been added to MT3DMS since v5 to save the calculated concentration at any observation point and the calculated mass flux at any sink/source location. The calculated values can be saved to output files along with the statistics of residuals between the calculated and observed values at the specified locations. The calculated concentrations can be interpolated from the neighboring nodal values if the observation point does not coincide with a model node. The calculated mass flux can be defined over any arbitrary group of sink/source cells referred to as a mass flux object.

3.2 IMPLEMENTING AND ACTIVATING THE TOB PACKAGE

The TOB Package is implemented in MT3DMS v5 by inserting the package name "TOB" into any unused slot of the "NameTRNOP" array in the MT3DMS main program, as illustrated below:

```
 DATA NameTRNOP/'ADV ', 'DSP ', 'SSM ', 'RCT ', 'GCG ',
&               '    ', '    ', '    ', '    ', '    ',
&               'TOB ', '    ', '    ', '    ', '    ',
&               '    ', '    ', '    ', '    ', '    '
```

To activate the TOB Package in a MT3DMS run, insert a line to the Name File of MT3DMS as shown below:

TOB   0   [project.tob]

where **TOB** is the input file type for the TOB Package; integer 0 is the default input unit number for the TOB Package (which is preset to 7 internally by MT3DMS); and `project.tob` is the name of the input file for the TOB Package.

An example of the MT3DMS Name File including the TOB Package:

```
#
# MT3DMS 5 Name File for test case P7
#

# Standard output file
LIST  0 p7.out

# Transport package input files
BTN    0 p7.btn
ADV    0 p7.adv
DSP    0 p7.dsp
SSM    0 p7.ssm
GCG    0 p7.gcg

# Transport observation input file
TOB    0 p7.tob

# Flow-Transport Link input file
FTL    0 p7.ftl  free noprint
```

3.3 INPUT INSTRUCTIONS

Input for the TOB Package is read from a file listed in the Name File with the keyword "TOB" as the file type. The input data are arranged and read sequentially in free format.

For Each Simulation

0.   [#Text]

Item 0 is optional and can include as many lines as desired. Each line needs to begin with the "#" character in the first column.

1.   MaxConcObs, MaxFluxObs, MaxFluxCells

2.   OUTNAM, inConcObs, inFluxObs, inSaveObs

9

Read items 3, 4, and 5 if [`inConcObs`] > 0

```
3.     nConcObs, CScale, iOutCobs, iConcLOG, iConcINTP

Read items 4 and 5 for [nConcObs] times
4.     COBSNAM, Layer, Row, Column, iComp, TimeObs, Roff,
       Coff, weight, COBS

Read item 5 if [Layer] < 0
5.     mLayer(1), prLayer(1), mLayer(2), prLayer(2), …,
       mLayer(|Layer|), prLayer(|Layer|)
```

Read items 6, 7, 8 and 9 if [`inFluxObs`] > 0

```
6.     nFluxGroup, FScale, iOutFlux

Read items 7, 8 and 9 for [nFluxGroup] times
7.     nFluxTimeObs, nCells, iSSType

Read item 8 [nFluxTimeObs] times
8.     FOBSNAM, iComp, FluxTimeObs, weight_fobs, FluxObs

Read item 9 [nCells] times for current mass flux object
9.     kcell, icell, jcell, factor
```

Text—is a character string (maximum of 79 characters) that starts in column 2. Any characters can be included in Text. The "#" character needs to be in column 1. Text is printed when the file is read and provides an opportunity for the user to include information about the model both in the input file and the associated output file.

MaxConcObs—is the maximum number of concentration observations allowed in the current simulation. This value is used for memory allocation purposes.

MaxFluxObs—is the maximum number of mass-flux observations. It should be set large enough to accommodate all mass-flux observations at different mass-flux objects and observation times. This value is used for memory allocation purposes.

MaxFluxCells—is the maximum number of model cells that makes up a mass-flux object. This value is used for memory allocation purposes.

OUTNAM—a string of one to 78 nonblank characters. OUTNAM specifies the base (root) name for three optional output files. The complete file names are composed of this base name followed by a period and a three-character extension listed below. The specification of lower and upper cases in OUTNAM is preserved in generating the file-name base. OUTNAM can include a path; constraints imposed by a particular computer operating system regarding file names and paths should be considered when specifying OUTNAM.

Output File	Content
`[OUTNAM].OCN`	Output file containing calculated concentrations, and optionally, residuals between the calculated and observed values, at user-defined observation points that are screened either in a single layer or across multiple layers. This text file is generated only if the flag `[inConcObs]` is greater than zero.
`[OUTNAM].MFX`	Output file containing calculated mass fluxes into or out of user-defined mass flux objects, and optionally, residuals between the calculated and observed values. Each mass flux object is defined by a group of model cells containing external sinks/sources such as wells, rivers, drains, recharge, and general-head boundaries. This text file is generated only if the flag `[inFluxObs]` is greater than zero.
`[OUTNAM].PST`	Output file containing calculated concentrations and mass fluxes at user-defined observation points and mass-flux objects. This output file, in binary form, is intended for post-processing purposes or for linkage with other modeling programs. This file is generated only if the flag `[inSaveObs]` is greater than zero.

inConcObs—is an integer flag indicating whether the calculated concentrations at the observation locations should be obtained and saved to the output file `[OUTNAM].OCN`. It also serves as the unit number for the output file `[OUTNAM].OCN`.

inFluxObs—is an integer flag indicating whether the calculated mass fluxes at the mass-flux objects should be obtained and saved to the output file `[OUTNAME].MFX`. It also serves as the unit number for the output file `[OUTNAM].MFX`.

inSaveObs—is an integer flag indicating whether the calculated concentrations and mass fluxes at the user-defined observation points and mass-flux objects should be saved to an unformatted (binary) output file `[OUTNAM].PST`. It also serves as the unit number for the output file `[OUTNAM].PST`.

nConcObs—is the number of concentration observations. Observations made at the same location but different times are considered multiple observations.

CScale—is the multiplier (scaling factor) for the observed concentrations. It is used to convert the unit of observed concentrations to the unit of calculated concentrations used internally in MT3DMS for computing appropriate residuals.

iOutCobs—is an integer flag indicating what type of output should be computed and saved:
iOutCobs = 0, calculated concentrations at the observation locations are saved to the output file [OUTNAM].OCN;
iOutCobs > 0, both calculated concentrations and residual errors between the calculated and observed values are saved to the output file [OUTNAM].OCN. The statistics of the residual errors is also computed and saved.

iConcLOG—is an integer flag indicating whether the calculated and observed concentrations should be converted to the common logarithm before computing the residual error and related statistics:
iConcLOG = 0, no conversion is done (residual error = calculated – observed);
iConcLOG > 0, convert the calculated and observed concentration values to the common logarithmic scale before computing the residual error and related statistics (residual error = $\log_{10}$Calculated – $\log_{10}$Observed).

iConcINTP—is an integer flag indicating whether the calculated concentration at an observation location should be interpolated from its neighboring nodal points, if the observation location does not coincide with a nodal point:
iConcINTP = 0, no interpolation is done (the calculated concentration value at the nearest nodal point is used for comparison with the observed value);
iConcINTP > 0, perform bilinear interpolation using four neighboring nodal concentrations in the same model layer.

COBSNAM—is a string of 1 to 12 nonblank characters used to identify the observation. The identifier need not be unique; however, identification of observations in the output files is facilitated if each observation is given a unique COBSNAM.

LAYER—is the layer index of the cell in which the concentration observation is located. If LAYER is less than zero, solute concentrations from multiple layers are combined to calculate a simulated value. The number of layers equals the absolute value of LAYER, or |LAYER|.

ROW—is the row index of the cell in which the concentration observation is located.

COLUMN—is the column index of the cell in which the concentration observation is located.

iComp—is an integer indicating the solute species for which the concentration observation is made. Integer 1 indicates the first species, 2 the second species, and so on.

TimeObs—is the time since the beginning of simulation to the time of the current observation. [TimeObs] should be included in the BTN input file as part of the input array [TIMPRS], i.e., the time to save simulation results. Otherwise, the calculated concentration is obtained from a time specified in [TIMPRS] or the end of a stress period that is closest to [TimeObs]. Note that if [TimeObs] is specified as a *negative* integer, the calculated concentration is saved whenever the number of transport steps is an even multiple of |TimeObs|.

Roff—is the row offset used to locate the observation within a finite-difference cell. The convention is the same as that used by MODFLOW-2000 (see Figure 3.1).

Coff—is the column offset used to locate the observation within a finite-difference cell. The convention is the same as that used by MODFLOW-2000 (see Figure 3.1).

weight—is the user-specified weighting factor for computing the residual error at the current observation, i.e., residual error = (calculated-observed)*weight. If [weight] is assigned a *negative* value, the observed concentration at the target observation point is not used and only the calculated concentration is saved.

COBS—is the concentration observation for the species defined by [iComp]. This input item is required regardless of whether the preceding input item [weight] has been given a positive or negative value.

mLayer(i)—is the ith layer number for a multilayer concentration observation.

prLayer(i)—is the proportion of the simulated solute concentration in layer mLayer(i) that is used to calculate a simulated multilayer concentration. The sum of all prLayer(i) values for a given observation needs to equal 1.0. The convention is the same as that used by MODFLOW-2000 (see Hill et al., 2000, p. 35). Note that if the concentration observation is made at a multi-node well (MNW), the flux-averaged composite concentration for the MNW wellbore can be computed and saved through the SSM Package for MT3DMS v5.

nFluxGroup—is the total number of mass flux objects. A mass flux object is defined as a group of model cells needed to represent one mass flux measurement.

FScale—is the multiplier (scaling factor) for the observed mass flux. It is used to convert the unit of observed mass flux to the unit of calculated mass flux observation used internally in MT3DMS for computing appropriate residuals.

COLUMNS

EXPLANATION

☐ Active cell   ▨ Inactive cell   ● Cell center   ○ Point
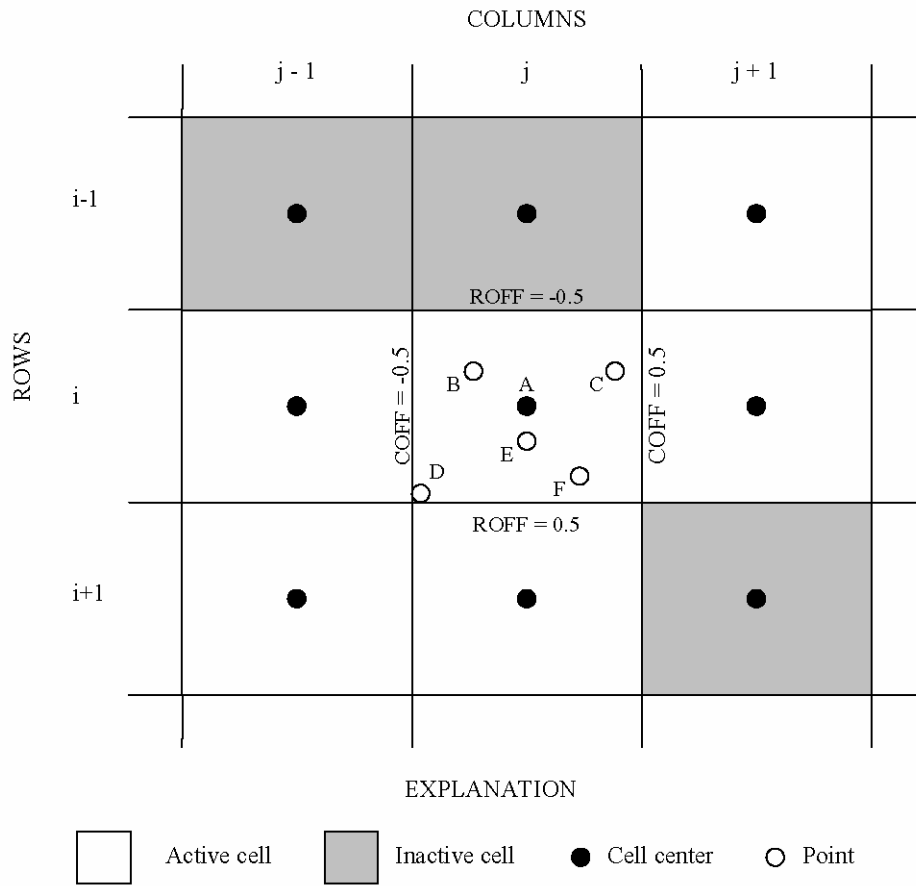
POINT	ROFF	COFF
A (Cell center)	0.0	0.0
B	-0.25	-0.25
C	-0.2	0.4
D	0.45	-0.45
E	0.25	0.0
F	0.4	0.25

Figure 3.1. Locating points within a finite-difference cell using ROFF and COFF (after Hill et al., 2000).

iOutFlux—is an integer flag indicating what type of output should be computed and saved:

iOutFlux = 0, calculated mass fluxes are saved to the output file `[OUTNAM].MFX`;

iOutFlux > 0, both calculated mass fluxes and residual errors between the calculated and observed values are saved to the output file `[OUTNAM].MFX`. The statistics of the residual errors is also computed and saved.

nFluxTimeObs—is the number of times at which mass fluxes are observed for the current mass-flux object.

nCells—is the total number of cells in the current mass-flux object.

iSSType—is an integer code indicating the type of sinks/sources constituting the current mass flux object. The [iSSType] codes used here are the same as those defined for the MT3DMS SSM Package:

iSSType Code	Type of Sink/Source
1	Constant-head
2	Well
3	Drain
4	River
5	Head-dependent boundary
6	(Reserved)
7	Recharge
8	Evapotranspiration
9-14	(Reserved)
15	Mass loading
21	Stream-routing
22	Reservoir
23	Specified flow and head boundary
24	Inter-bed storage
25	Transient leakage
26	Lake
27	Multi-node well
28	Drain with return flow
29	Segmented evapotranspiration
30-49	(Reserved)
50	HSSM-LNAPL
51	User-defined #1
52	User-defined #2
53	User-defined #3

FOBSNAM—is a string of 1 to 12 nonblank characters used to identify the mass flux observation. The convention is the same as that for COBSNAM. The first part of FOBSNAM can be used to identify a common group name, while the rest to distinguish different observations for the same group.

FluxTimeObs—is the time since the beginning of simulation to the time of the current mass flux observation. [FluxTimeObs] should be included in the BTN input file as part of the input array [TIMPRS], i.e., the time to save simulation results. Otherwise, the calculated mass flux is obtained from a time specified in [TIMPRS] or the end of a stress period that is closest to [FluxTimeObs]. Note that if [FluxTimeObs] is specified as a *negative* integer, the calculated mass flux is saved whenever the number of transport steps is an even multiple of |FluxTimeObs|.

weight_fobs— is the user-specified weighting factor for computing the residual error at the current mass-flux object, i.e., residual error = (calculated-observed)*weight. If [weight_fobs] is assigned a *negative* value, the observed mass flux at the target mass-flux object is not used and only the calculated mass flux is saved.

FluxObs—is the observed solute mass flux, QC [dimension, MT^{-1}], for the user-specified species [iComp]. The mass flux observation is negative when the mass is leaving the groundwater system, and positive when the mass is entering the groundwater system. This input item is required regardless of whether the preceding input item [weight_fobs] has been given a positive or negative value.

kcell—is the layer index of a sink/source cell included in the current mass flux object.

icell—is the row index of a sink/source cell included in the current mass flux object.

jcell—is the column index of a sink/source cell included in the current mass flux object.

factor—is the weighting factor for the mass flux calculated at the specified cell location (jcell, icell, kcell). [factor] = 1.0 under most circumstances, i.e., the specified cell belongs to a single mass-flux object. However, the mass flux calculated at one specific cell can be assigned to one or more mass-flux objects that cover portions of the cell. In that case, [factor] can be less than 1.0. Regardless, the sum of [factor] values at a single cell for multiple mass-flux objects should add up to 1.0.

3.4 OUTPUT INFORMATION

As pointed out previously, three optional output files may be created depending on how the output options are specified in the input file to the TOB Package. These files are

1) a text file with the 3-letter extension ".OCN" which contains the calculated concentrations, and if requested, the residuals between the calculated and

observed values, at the user-specified observation locations. This text file is generated only if the concentration observation flag [inConcObs] is specified in the TOB input file as greater than zero.

2) a text file with the 3-letter extension ".MFX" which contains the calculated mass fluxes into or out of user-defined mass flux objects, and if requested, the residuals between the calculated and observed values. Each mass flux object is defined by a group of model cells containing external sinks/sources such as wells, rivers, drains, recharge, and general-head boundaries. This text file is generated only if the mass flux observation flag [inFluxObs] is specified in the TOB input file as greater than zero.

3) an unformatted (binary) file with the 3-letter extension ".PST" which contains the calculated concentrations and/or mass fluxes at user-defined observation points.

The records in the PST binary output file are in the form of
[cobsnam, TimeObs, CCal]
for concentration observations where cobsnam is the name of the concentration observation as a string of 12 characters , and TimeObs and CCal are real numbers indicating the observation time and the calculated concentration value.

The records in the PST binary output file are in the form of
[fobsnam, TimeFluxObs, FluxCal]
for mass-flux observations where fobsnam is the name of the mass-flux observation as a string of 12 characters , and TimeFluxObs and FluxCal are real numbers indicating the observation time and the calculated mass flux.

This output file is intended for post-processing purposes or for linkage with other modeling programs. The file is generated only if the output flag [inSaveObs] is specified in the TOB input file as greater than zero.

4 Simulating the Effect of Multi-Node Wells on Solute Transport

4.1 BACKGROUND

Halford and Hanson (2002) developed the drawdown-limited, Multi-Node Well (MNW) Package for MODFLOW. The MNW Package allows MODFLOW users to simulate wells that are screened in multiple aquifers or multiple layers in a single aquifer, and multiple nodes in a horizontal well. A MNW dynamically distributes the total prescribed flow among different layers (or nodes) under either extraction or injection conditions. In addition, intra-wellbore flow between layers are computed under zero-pumping conditions. A single hydraulic head value is determined for the entire wellbore. Although the MNW Package also has the ability to track potential mixes of a water-quality attribute, it is based on the prescribed constant concentrations and does not consider solute transport.

MT3DMS v5 adds the capability to simulate the effect of multi-aquifer or multi-node wells on solute transport. Compatible with the MNW Package, MT3DMS v5 computes a single composite concentration for the entire well borehole based on the flux-weighted concentrations of the injected fluid (if any) and the flow rates from different layers. The average composite concentration at the wellbore at any time is computed from:

$$C_{avg}^t = \frac{\left|Q_w^t\right|C_w^t + \sum_{i=1}^N \left|Q_i^t\right|C_i^t}{\left|Q_w^t\right| + \sum_{i=1}^N \left|Q_i^t\right|}$$

(4.1)

where

C_{avg}^t is the flux-averaged composite concentration inside the wellbore at time t;

Q_w^t is the total prescribed flow **into** the multi-node well (i.e., source) at time t;

C_w^t is the concentration of the injected source Q_w^t at time t;

Q_i^t is the flow rate at node (layer) i **discharging** into the multi-node well (i.e., sink) at time t;

C_i^t is the concentration associated with the sink outflow Q_i^t, i.e., the
concentration in the aquifer at node (layer) i at time t; and

N is the total number of nodes (layers) that makes up the multi-node well.

It is noteworthy that the single composite concentration C_{avg}^t inside the wellbore is the actual concentration of the inflow that may go into individual nodes (layers) over which the multi-node well is screened. Further note that even if the total prescribed Q_w^t is zero, i.e., the multi-node well is under zero injection or pumping conditions, there is still potential intra-wellbore flow from layers (nodes) with higher heads to those with lower heads. Correspondingly, mass exchange may occur due to the intra-wellbore flow.

4.2 INPUT INSTRUCTIONS

To simulate the effect of multi-node wells on solute transport, the MNW Package must have been used with MODFLOW-2000 to save the sink/source information in the Flow-Transport link file that is produced after a MODFLOW-2000 run. Although the MNW Package can be used with both MODFLOW-96 and MODFLOW-2000, only version 6.2 or later of the Link-MT3DMS (LMT6) Package added to MODFLOW-2000 since version 1.12 (dated 9/8/2003) has the capability to save the MNW flow term for use by MT3DMS v5.

The input file for the LMT6 Package of MODFLOW-2000 must have the **OUTPUT_FILE_HEADER** option set to **"EXTENDED"**, as shown below:

```
OUTPUT_FILE_NAME      project.ftl
OUTPUT_FILE_UNIT      333
OUTPUT_FILE_HEADER    extended
OUTPUT_FILE_FORMAT    unformatted
```

which instructs MODFLOW-2000 to save the MNW flow term correctly in the flow-transport line file. For more information on the LMT6 Package, refer to Zheng et al. (2001).

If a MNW is a sink (extracting water from the well), it is not necessary to specify a concentration for the MNW. If assigned, it will be ignored anyway. A single composite concentration for all layers within a MNW is determined internally based on equation (1). If a MNW is a source (injecting water into the well), the user may specify any desired concentration for the MNW source. If it is not specified a concentration, the source is assumed, by default, to have a zero concentration. Also, regardless of how many layers (nodes) a MNW may be screened over, it is only necessary to assign the concentration for just one layer (node) within the wellbore of the MNW (all layers or nodes are equivalent). For a MNW under zero pumping or injection conditions, there is nothing to specify.

The input record for specifying the source concentration for a multi-node well in the SSM Package input file is as follows:

For Single-Species Simulation:

Record: K, I, J, CSS, iSSType
Format: 3I10, F10.0, I10

For Multi-Species Simulation:

Record: K, I, J, CSS, iSSType, (CSS(index),index=1,ncomp)
Format: 3I10, F10.0, I10, free

where I and J are the horizontal locations (row and column) and K is the vertical location (layer) of the MNW over which the MNW is screened. CSS is the source concentration if only a single species is simulated. For multi-species simulations, specify one concentration for each of NCOMP species. iSSType is the sink/source type code for MNW. The integer code of iSSType is 27 for MNW.

An example of the SSM input file with the MNW source:

```
HEADER_LINE     [dummy input, not used by MT3DMS v5]
    1000        [MXSS: Max # of Sinks/Sources]
       1        [NSS: # of point sources with specified conc.]
       1    24        24      100.        27    [K,I,J,CSS,iSSType]
```

In the above example, the multi-node well (iSSType=27) is located at two or more model cells, one of which must be at layer K=1, row I=24, and column J=24 with an input concentration of CSS=100. The total prescribed flow to the multi-node well is saved in the Flow-Transport link file produced by MODFLOW-2000.

4.3 OUTPUT INFORMATION

The location and the internally-determined composite concentration for each MNW is saved to the MT3DMS standard text output file generated after each run. The results are saved only at the end of each stress period or at the times specified by the user in the BTN input file. Alternatively, the user can specify a unit number for a MNW-specific output file. This unit can be specified in the second input record of the SSM input file as illustrated below:

Record: MXSS, ISSGOUT
Format: 2I10

where the input value $\mathtt{ISSGOUT}$ is the unit number for the MNW-specific output file. $\mathtt{ISSGOUT}$ must be a unique integer that has not be used elsewhere. After $\mathtt{ISSGOUT}$ is specified, a new line must be inserted to the Name File for the MT3DMS run, as follows:

```
DATA    ISSGOUT    OuputFileName
```

where $\mathtt{DATA}$ is the keyword not to be modified and $\mathtt{OutputFileName}$ is the user-specified name for the file to which the location and the internally-determined composite concentration of each MNW will be saved at every transport step.

5 Support for Additional MODFLOW-2000 Sink/Source Packages

In addition to the MNW Package, MT3DMS v5 provides the support for two more MODFLOW sink/source packages, i.e., the Drain with Return Flow (DRT) and Evapotranspiration with Segments (ETS), both documented in Banta (2000). Table 5.1 is an updated list of MODFLOW-2000 flow and sink/source packages and their support status in MT3DMS v5 (the bold typeface indicates those packages newly supported in this version). Interested users should refer to the README file distributed with other MT3DMS distribution files at the MT3D website for the most up-to-date information on the support status of other add-on packages to MODFLOW-2000.

The DRT Package simulates the re-injection of all or a portion of the outflow from a drain back into the aquifer. MT3DMS v5 automatically assigns the concentration at the outflow cell as that of the re-injected source at the return location. The user can specify the proportion of the return drain flow in the DRT input file to MODFLOW, but cannot alter the concentration of the return drain flow, which is controlled by the concentration in the aquifer. The DRT Package is useful in some applications, such as the use of aquifer water discharged into certain drain features directly for agricultural irrigation without any alternation to the water quality.

The ETS Package allows simulation of evapotranspiration with a user-defined relation between evapotranspiration rate and hydraulic head. The ETS provides additional capability and flexibility not available in the EVT Package, which has been available in MODFLOW since its initial release. In MT3DMS v5, the sink flow term produced by the ETS is handled exactly the same way as that produced by the EVT Package. Thus the input instructions for the EVT flow sink (Zheng and Wang, 1999) are directly applicable to the ETS flow sink.

It is noteworthy that in an effort to maintain backward compatibility with previous versions of MT3DMS, the Flow-Transport Link file produced by MODFLOW-2000 has two header options, **"standard"** and **"extended"** (see Zheng et al., 2001). As pointed out previously for the MNW Package, the header option of the Flow-Transport Link file must be set to **"extended"** in the input file to the Link-MT3DMS (LMT6) Package of MODFLOW-2000 for the flow terms of the DRT and ETS Packages to be saved appropriately for use in MT3DMS v5. This is also true for any subsequent MODFLOW-2000 sink/source packages that will be supported in the future.

The structure and contents of the Flow-Transport Link file used by MT3DMS v5 are specified in the Link-MT3DMS (LMT6) Package version 6.2 implemented in MODFLOW-2000 since version 1.12. Developers who wish to add support for a specific MODFLOW sink/source package should follow the same conventions and make appropriate changes to the Flow-Model-Interface (FMI) Package of MT3DMS. Use the pre-defined iSSType code if a sink/source type has been already defined in MT3DMS (Table 5.1). If not, use any unique integer code up to the maximum value of 100.

Table 5.1. List of MODFLOW packages and their support status by MT3DMS v5.

MODFLOW Package Name (documented in Harbaugh and others, 2000, or in references cited in that work)	File Type of MODFLOW-2000 Name File	MT3DMS iSSType Code for Sinks/Sources	Support Status in MT3DMS v5
Basic	BAS6	n/a	Yes
Block-Centered Flow	BCF6	n/a	Yes
Layer Property Flow	LPF1	n/a	Yes
Hydrogeologic Unit Flow	HUF2	n/a	Yes
Horizontal Flow Barrier	HFB	n/a	Yes
Time-Variant Specified Head Boundary	CHD	1	Yes
Well	WEL	2	Yes
Drain	DRN	3	Yes
River	RIV	4	Yes
General Head Dependent Boundary	GHB	5	Yes
Recharge	RCH	7*	Yes
Evapotranspiration	EVT	8*	Yes
Streamflow-Routing	STR	21	Yes
Reservoir	RES	22	Yes
Specified Flow and Head Boundary	FHB	23	Yes
Interbed Storage	IBS	24	No
Transient Leakage	TLK	25	No
Lake	LAK	26	No
Multi-Node Well	**MNW**	**27**	**Yes**
Drain with Return Flow	**DRT**	**28**	**Yes**
Evapotranspiration with Segments	**ETS**	**29**	**Yes**

*Note: these codes are for identification purposes only. Recharge and Evapotranspiration are considered areally distributed sinks/sources rather than point sinks/sources.

6 Simulating Zeroth-Order Reactions in Single- and Dual-Domain Systems

6.1 BACKGROUND

The standard MT3DMS code prior to version 5 includes only the first-order kinetic reactions in the Chemical Reaction (RCT) Package. However, zeroth-order reactions may be useful for describing certain types of biogeochemical decay or production. In addition, zeroth-order reactions are needed in direct simulation of groundwater ages (e.g., Goode, 1996) and calculation of parameter sensitivities (e.g., Tsai et al., 2003). Thus since version 5.1, zeroth-order reactions have been added to the Chemical Reaction Package in both single- and dual-domain formulations.

The governing solute transport equations incorporating the zeroth-order decay or production terms in both dissolved and sorbed phases can be written as

For equilibrium-controlled sorption

$$R\frac{\partial(\theta C)}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(q_i C) + q_s C_s - \gamma_1\theta - \gamma_2\rho_b \qquad (6.1)$$

For rate-limited kinetic sorption

$$\frac{\partial(\theta C)}{\partial t} + \frac{\partial(\rho_b\overline{C})}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(q_i C) + q_s C_s - \gamma_1\theta - \gamma_2\rho_b \qquad (6.2a)$$

$$\frac{\partial(\rho_b\overline{C})}{\partial t} = \beta\left(C - \frac{\overline{C}}{K_d}\right) - \gamma_2\rho_b \qquad (6.2b)$$

where γ_1 and γ_2 are the zeroth-order rate coefficients for the dissolved phase [ML^{-3}T^{-1}], and the sorbed phase [MM^{-1}T^{-1}], respectively. The conventions for both γ_1 and γ_2 are *positive values for decay* and *negative values for production*. Other terms in equations (6.1) and (6.2) have been defined in Zheng and Wang (1999), i.e., C is the dissolved concentration [ML^{-3}]; θ the porosity, dimensionless; D_{ij} the hydrodynamic dispersion coefficient tensor [L^{2}T^{-1}]; q_i the specific discharge (Darcy flux) [LT^{-1}]; q_s the volumetric flow rate per unit volume of aquifer representing fluid sources (positive) or sinks (negative) [T^{-1}]; C_s the concentration of the fluid source or sink [ML^{-3}]; ρ_b the

bulk density of the subsurface medium [ML^{-1}]; $\overline{C}$ the sorbed concentration [MM^{-1}]; K_d the distribution coefficient of linear sorption isotherm [L^{3}M^{-1}]; R the retardation factor [dimensionless]; and β the first-order rate coefficient between the dissolved and sorbed phases [T^{-1}].

In a dual-domain (dual-porosity) system, the governing transport equations incorporating linear equilibrium-controlled sorption and zeroth-order reactions can be written as

$$R_m \frac{\partial(\theta_m C_m)}{\partial t} + R_{im} \frac{\partial(\theta_{im} C_{im})}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta_m D_{ij} \frac{\partial C_m}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(q_i C_m) + q_s C_s \qquad (6.3a)$$

$$- \gamma_{1,m}\theta_m - \gamma_{1,im}\theta_{im} - \gamma_{2,m}f\rho_b - \gamma_{2,im}(1-f)\rho_b$$

$$R_{im} \frac{\partial(\theta_{im} C_{im})}{\partial t} = \zeta(C_m - C_{im}) - \gamma_{1,im}\theta_{im} - \gamma_{2,im}(1-f)\rho_b \qquad (6.3b)$$

where C_m and C_{im} are the dissolved concentrations in the mobile and immobile domains, respectively [ML^{-3}]; θ_m and θ_{im} are the porosities of the mobile and immobile domains, respectively [dimensionless]; $\gamma_{1,m}$ and $\gamma_{1,im}$ are the zeroth-order rate coefficients for the mobile-liquid and immobile-liquid phases, respectively [ML^{-3}T^{-1}]; $\gamma_{2,m}$ and $\gamma_{2,im}$ are the zeroth-order rate coefficients for the mobile-sorbed and immobile-sorbed phases, respectively [ML^{-3}T^{-1}]; f is the fraction of sorption sites in contact with the mobile fluid phase [dimensionless]; $R_m = 1 + f\rho_b K_d/\theta_m$ and $R_{im} = 1 + (1-f)\rho_b K_d/\theta_{im}$ are the retardation factors for the mobile and immobile domains, respectively [dimensionless]; and ζ is the first-order mass transfer rate coefficient between the mobile and immobile domains [T^{-1}].

6.2 IMPLEMENTATION AND INPUT INSTRUCTIONS

The implementation of zero-order reactions in MT3DMS is done similar to that of first-order reactions. The contributions from the zero-order reactions are directly incorporated into the coefficient matrix [A] and the right-hand-side matrix [RHS] of the linear system of equations resulting from the various solution schemes for the transport model (Zheng and Wang, 1999). In addition, the formulation for the concentration of sorbed phase or immobile-liquid phase is updated to account for the effect of zero-order reactions.

To invoke the zeroth-order reaction option, set the input variable IREACT = **100** in the input file for the RCT Package (see Appendix A). Then, in the input records where the user would normally enter the first-order rate coefficients RC1 for the dissolved phase and RC2 for the sorbed phase, specify the zeroth-order rate coefficients. When sorption is not simulated, set the input variable RC2 to zero. Even though RC2 is not used when sorption is not present, it nevertheless must be specified in the input file.

6.3 BENCHMARK TEST PROBLEMS

6.3.1. Zero-Order Production in a Uniform Flow Field

This benchmark problem involves solute transport in a uniform flow field in the presence of zero-order production. The initial condition for the one-dimensional problem is defined by zero concentration everywhere in the flow field, i.e.,

$$C(x,0) = 0 \qquad x \geq 0 \qquad\qquad (6.4)$$

and the boundary conditions are specified mass flux (third-type) on the left and specified concentration gradient on the right:

$$qC - D\frac{\partial C}{\partial x}\bigg|_{x=0} = \begin{cases} q_0 C_0 & 0 < t \leq t_0 \\ 0 & t > t_0 \end{cases}$$

$$\frac{\partial C}{\partial x}\bigg|_{x=\infty} = 0, \qquad t > 0 \qquad\qquad (6.5)$$

A flow and transport model consisting of 101 columns, 1 row and 1 layer is set up to solve the test problem. Other parameters used for the test problem are listed below:

Cell width along rows (Δx) = 0.16 m
Cell width along columns (Δy) = 1 m
Layer thickness (Δz) = 1 m
Seepage velocity (v) = 0.1 m/day
Longitudinal dispersivity = 1.0 m
Porosity (θ) = 0.37
Zeroth-order rate coefficient (γ_1) = 2×10^{-3} mg/L day^{-1}
Pulse source duration (t_o) = 160 days
Simulation time (t) = 1,000 days
Observation location (x) = 8 m

The numerical solution is obtained using the fully implicit finite-difference option for all transport terms. The transport step size is fixed at 1 day for ease of comparison. The relative concentration closure criterion for the GCG matrix solver is set at 10^{-6} and the MIC pre-conditioner is selected.

Figure 6.1 shows the concentration breakthrough curve at the observation point as calculated by MT3DMS (symbols). A corresponding analytical solution is available from Toride et al. (1995) (solid line). It is evident that the numerical solution by MT3DMS closely agrees with the analytical solution of Toride et al. (1995).
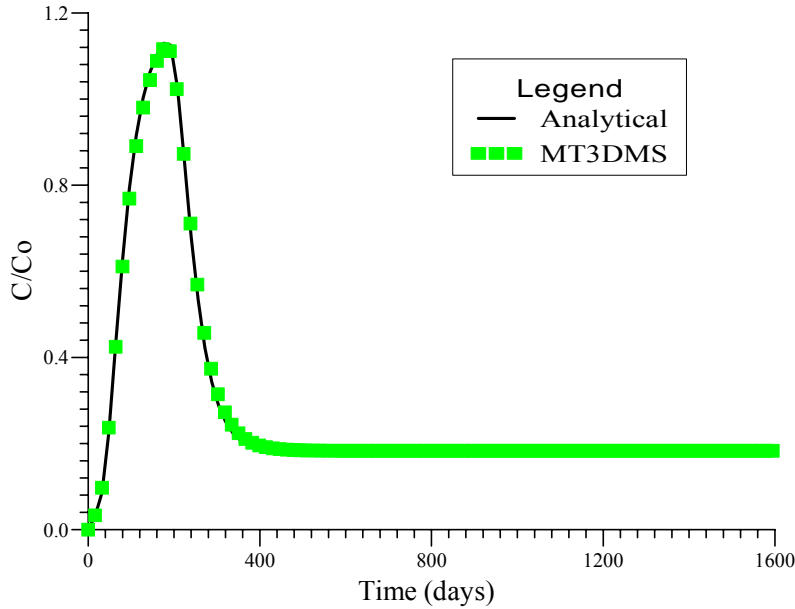
Figure 6.1. Comparison of analytical and numerical solutions for the test problem with zeroth-order reaction.

6.3.2. Zero-Order Production in a Dual-Domain System

This benchmark problem is designed to test the capabilities of MT3DMS to simulate solute transport in a dual-domain system in the presence of zero-order production with or without linear sorption. A general analytical solution for one-dimensional solute transport in a dual-domain system, implemented in the computer code CXTFIT2, is available from Toride et al. (1995). The one-dimensional problem considered in this section involves the following initial condition for both mobile-liquid and immobile-liquid phases:

$$C(0,0) = C_0$$
$$C(x,0) = 0 \qquad x > 0 \tag{6.6}$$

and a first-type (constant-concentration) boundary condition on the left and a second-type (constant concentration gradient) on the right:

$$C(0,t) = \begin{cases} C_0 & 0 < t \le t_0 \\ 0 & t > t_0 \end{cases}$$

$$\frac{\partial C(\infty, t)}{\partial x} = 0 \qquad t > 0 \tag{6.7}$$

A numerical flow and transport model consisting of 401 columns, 1 row and 1 layer is used to solve the problem for comparison with the analytical solution for the same initial and boundary conditions as described above. In the flow model, the first and last columns are constant-head boundaries. Arbitrary hydraulic heads are used to

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establish the required uniform hydraulic gradient. In the transport model, the first column is a constant-concentration boundary with a relative concentration of one. The last column is set sufficiently far away from the source to approximate an infinite one-dimensional flow domain as assumed in the analytical solution. The model parameters used in the simulation are listed below:

Cell width along rows (Δx) = 2.5 m

Cell width along columns (Δy) = 1 m

Layer thickness (Δz) = 1 m

Specific discharge (q) = 0.06 m/day

Longitudinal dispersivity = 10 m

Porosity of mobile domain (θ_m) = 0.2

Porosity of immobile domain (θ_{im}) = 0.05

Bulk density (ρ_b) = 4 g/mL

Distribution coefficient (K_d) = 0.25 mL/g

First-order mass transfer rate between
the mobile and immobile domains (ζ) = 10^{-3} day^{-1}

Fraction of sorption sites
in contact with mobile water (f) = 0.8

Source duration (t_0) = 1,000 days

Simulation time (t) = 10,000 days

Observation location (x) = 200 m

Three cases are evaluated with the following zero-order production coefficients and retardation factors:

Case 1: $R_m = R_{im} = 5$, $\gamma_1 = 0$; $\gamma_2 = 10^{-3}$ g/mL day^{-1};

Case 2: $R_m = R_{im} = 5$; $\gamma_1 = \gamma_2 = 5 \times 10^{-4}$ g/mL day^{-1};

Case 3: $R_m = R_{im} = 1$ $(K_d = 0)$; $\gamma_1 = 10^{-3}$ g/mL day^{-1}; $\gamma_2 = 0$.

where Case 3 is equivalent to no sorption.

By default it is assumed in MT3DMS that the fraction of sorption sites in contact with mobile water (f) is equal to the ratio of mobile to total porosities so that the retardation factor for the mobile domain is identical to that for the immobile domain. In addition, it is assumed that the rate constant for the zero-order production is the same for both mobile and immobile domains, i.e., $\gamma_1 = \gamma_{1,m} = \gamma_{1,im}$ and $\gamma_2 = \gamma_{2,m} = \gamma_{2,im}$. However, different rate constants can be specified for the dissolved (liquid) and solid (sorbed) phases.

All cases are solved using the third-order TVD scheme for the advection term and the fully implicit finite-different option for all other terms. The closure criterion for the GCG solver is set at 10^{-6} and the MIC pre-conditioner is selected. For ease of comparison, a fixed transport step size of 1 day is used for all cases.

A close match between the analytical (solid lines) and numerical solutions (symbols) is obtained for all cases (Figure 6.2). Note that only the concentrations of the mobile-liquid phase are plotted. Other three phases, i.e., mobile-sorbed, immobile-liquid, and immobile-sorbed, are tracked internally by MT3DMS that also computes and maintains a global mass budget for all four phases. Negligible mass balance errors are obtained for all the cases considered in this example.
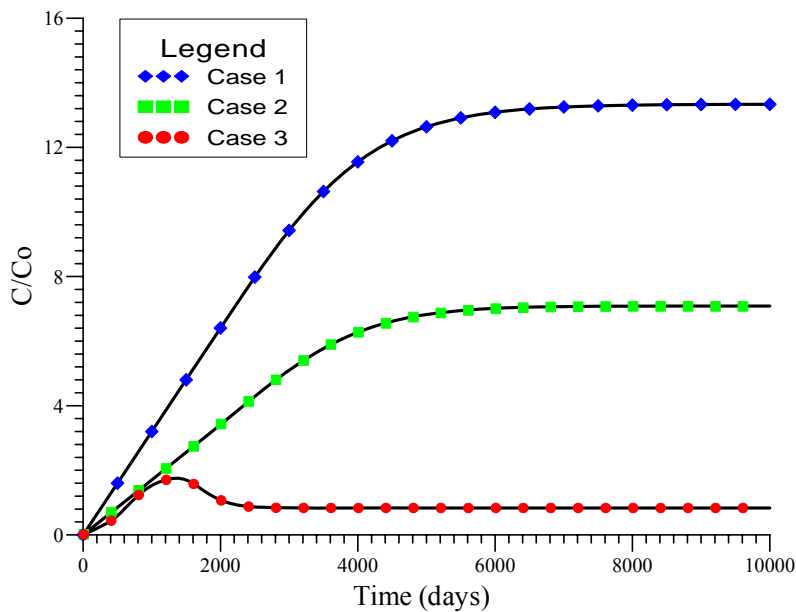

Fig. 6.2. Comparison of the calculated concentrations with the analytical solutions for the one-dimensional dual-domain test problem. The analytical solutions are shown in solid lines with the numerical solutions in different symbols. The reaction parameters for the 3 cases are given in the text.

7 Using the Multicomponent Diffusion Option

7.1 BACKGROUND

Prior to Version 5.2, the molecular diffusion coefficient can only be specified on a layer-by-layer basis (i.e., one uniform molecular diffusion coefficient for the entire model layer). Moreover, all solute components are assumed to have the same diffusion coefficient. However, in a multicomponent simulation, it is possible that different ions and solutes may have noticeably different molecular diffusion coefficients. In addition, the molecular diffusion coefficient may also vary spatially in each layer of the model domain. Thus a new option has been added to Version 5.2 to allow the inclusion of three-dimensional multicomponent diffusion coefficients in the transport simulation. The option is implemented through the Dispersion (DSP) Package and the modifications made to the MT3DMS code are limited to within the DSP Package only.

7.2 INPUT INSTRUCTIONS

To activate the *multicomponent diffusion* option, a keyword input record must be inserted to the beginning of the Dispersion (DSP) input file. The symbol $ in the *first* column of an input line signifies a keyword input record containing one or more predefined keywords. Above the keyword input record, comment lines marked by the symbol # in the first column are allowed. Comment lines are processed but have no effect on the simulation. Furthermore, blank lines are also acceptable above the keyword input record. Below the keyword input record, the format of the DSP input file must remain unchanged from the previous versions except for the diffusion coefficient as explained below. If no keyword input record is specified, the input file remains backward compatible with all previous versions of MT3DMS.

The predefined keyword for the multicomponent diffusion option is **MultiDiffusion**. The keyword is case insensitive so "MultiDiffusion" is equivalent to either "Multidiffusion" or "multidiffusion". If this keyword is specified in the keyword input record that has been inserted into the beginning of the DSP input file, the multicomponent diffusion option has been activated and the user needs to specify one diffusion coefficient for *each mobile solute component* and *at each model cell*. This is done by specifying one mobile component at a time, from the first component to the last component (MCOMP). For each mobile component, the real array reader utility (RARRAY) is used to input the 3-D diffusion coefficient array, one model layer at a time. Given below in Table 7.1 is an example of the Dispersion Package input file with the multicomponent diffusion option activated.

Table 7.1. An example DSP input file with the multicomponent diffusion option.

```
#
# DSP input file with keyword line indicated by $ sign in column 1
#
$ MultiDiffusion
        0       10.                             AL-LAYER 1
        0       10.                             AL-      2
        0       10.                             AL-      3
        0       10.                             AL-      4
        0       10.                             AL-      5
        0       10.                             AL-      6
        0       10.                             AL-      7
        0       10.                             AL-      8
        0        .3                             TRPT
        0        .3                             TRPV
        0       1.0                             DMCOEF  L1 Comp-1
        0       1.0                             DMCOEF  L2
        0       1.0                             DMCOEF  L3
        0       1.0                             DMCOEF  L4
        0       1.0                             DMCOEF  L5
        0       1.0                             DMCOEF  L6
        0       1.0                             DMCOEF  L7
        0       1.0                             DMCOEF  L8
        0        .0                             DMCOEF  L1 Comp-2
        0        .0                             DMCOEF  L2
        0        .0                             DMCOEF  L3
        0        .0                             DMCOEF  L4
        0        .0                             DMCOEF  L5
        0        .0                             DMCOEF  L6
        0        .0                             DMCOEF  L7
        0        .0                             DMCOEF  L8
        0        .1                             DMCOEF  L1 Comp-3
        0        .1                             DMCOEF  L2
        0        .1                             DMCOEF  L3
        0        .1                             DMCOEF  L4
        0        .1                             DMCOEF  L5
        0        .1                             DMCOEF  L6
        0        .1                             DMCOEF  L7
        0        .1                             DMCOEF  L8
```

8 Simulating the Effect of a Recirculation Well

A new option has been added to MT3DMS since Version 5.2 to simulate the effect of a recirculation well on solute transport. A recirculation well is defined as an injection well whose input concentration is equal to the output concentration of an extraction well. This option is implemented in the Sink/Source Mixing (SSM) Package for the type-2 point sources, i.e., injection wells.

To use the *recirculation well* option, set the input concentration (CSS) of the injection well to an negative integer code (IC), i.e.,

$$CSS = -IC$$

with the absolute value of the integer code (IC) given as

$$IC = NCOL \times NROW \times (K-1) + NCOL \times (I-1) + J$$

where NCOL and NROW are the total numbers of columns and rows, respectively, in the model; and K, I, J are the layer, row, and column indexes of the model cell (extraction well) whose concentration is to be used as the input concentration of the recirculation well. For a multicomponent simulation, the IC value must be specified for the concentrations of different components [CSSMS].

As an example, let's assume an extraction well at K = 1, I = 16, and J = 21 (see Figure 8.1). The total numbers of layers, rows and columns in the model are NLAY = 1, NROW = 31 and NCOL = 46. Now let's specify two recirculation wells, one at (K, I, J) = (1, 5, 16) and the other at (K, I, J) = (1, 27, 16). The input concentration to both recirculation wells should be the same as that of the extraction well at (K, I, J) = (1, 16, 21). The IC value for both recirculation wells is

$$IC = 46 \times 31 \times (1-1) + 46 \times (16-1) + 21 = 711$$

Thus to specify the two recirculation wells for the MT3DMS SSM Package, we have

K	I	J	CSS	ISSType
1	5	16	-711	2
1	27	16	-711	2

where K, I, J are the location indexes of the recirculation wells and ISSType is the MT3DMS sink/source type code (ISSTYPE=2 for the well).

Note that to obtain an accurate solution for the recirculation well option, it is suggested that the maximum outer iteration number of the GCG solver be set to greater than 1 to ensure the concentrations at the extraction and recirculation wells have converged during the iterations.
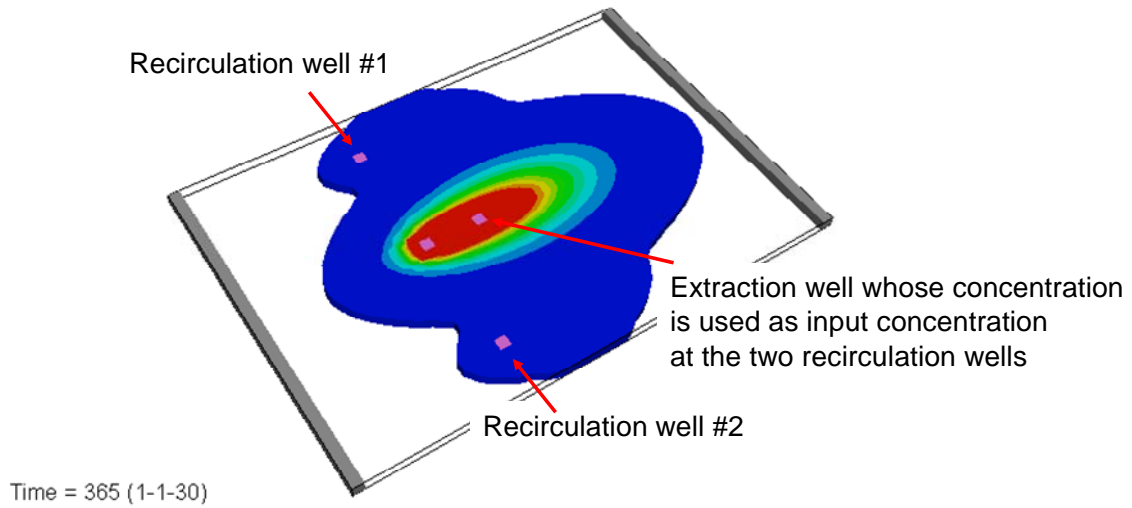
Recirculation well #1

Extraction well whose concentration is used as input concentration at the two recirculation wells

Recirculation well #2

Time = 365 (1-1-30)

Figure 8.1. Illustration of the recirculation well option.

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Appendix A
Changes to the Input Instructions since MT3DMS v5.0

I. CHANGES FOR THE BTN PACKAGE

Prior to version 5.0

    A5   Record: TRNOP(10)
               Format: 10L2
- TRNOP contains logical flags (true or false) for major transport and solution options.

Changes since version 5.0

    A5   Record: Dummy input line
               Format: n/a
- TRNOP is no longer used since MT3DMS v5.0. However, a dummy input line must still be specified in the input file. A blank line is acceptable.

II. CHANGES FOR THE DSP PACKAGE

Prior to version 5.2

C1   Array: AL(NCOL,NROW)   (One array for each layer).
       Reader: RARRAY
               • AL is the longitudinal dispersivity, α_L, for every cell of the model grid (unit: L).

……
C4   Array: DMCOEF(NLAY)
       Reader: RARRAY
               • DMCOEF is the effective molecular diffusion coefficient (unit: L^2T^{-1}). Set DMCOEF = 0 if the effect of molecular diffusion is considered unimportant. Each value in the array corresponds to one model layer.

Changes since version 5.2

C0   Record: One or more optional keywords.
       Format: [Free]
               • The only keyword currently supported is **MultiDiffusion**, case insensitive. **The keyword must be specified in an input line with the $ sign in the first column**. The keyword input record is optional.

C1   Array: AL(NCOL,NROW)   (One array for each layer).
       Reader: RARRAY
               • No change.

……
If no keyword is defined:
C4   Array: DMCOEF(NLAY)
       Reader: RARRAY
               • DMCOEF is the effective molecular diffusion coefficient (unit: L^2T^{-1}). Set DMCOEF = 0 if the effect of molecular diffusion is considered unimportant. Each value in the array corresponds to one model layer. **Enter one array for all solute components.**

If keyword [MultiDiffusion] is defined:
C4   Array: DMCOEF(NCOL,NROW)   (One array for each layer)
       Reader: RARRAY
               • DMCOEF is the effective molecular diffusion coefficient (unit: L^2T^{-1}). Set DMCOEF = 0 if the effect of molecular diffusion is considered unimportant. Each value in the array corresponds to one model cell. **Repeat the input for each mobile component.**

III. CHANGES FOR THE SSM PACKAGE

<u>Prior to version 5.0</u>

D1   Record: FWEL, FDRN, FRCH, FEVT, FRIV, FGHB, (FNEW(n), n=1,4)
          Format: 10L2
- These are logical flags (true or false) to indicate whether various MODFLOW sink/source packages are used in the flow simulation.

<u>Changes since version 5.0</u>

D1   Record: Dummy input line
          Format: n/a
- These logical flags are no longer needed as the status of various flow sink/source packages is obtained by MT3DMS through the Flow-Transport Link File produced by MODFLOW. However, a dummy input line must still be specified in the input file. A blank line is acceptable.

<u>Prior to version 5.0</u>

D2   Record: MXSS
          Format: I10
- MXSS is the maximum allowed number of all point sinks and sources included in the flow model. This input value is used for the memory allocation purpose only.

<u>Changes since version 5.0</u>

D2   Record: MXSS, **ISSGOUT**
          Format: 2I10
- ISSGOUT is the unit number for an optional output file to save the calculated flux-averaged composite concentrations at multi-node wells. The name of the output file must be specified through the Name File as in **"DATA   ISSGOUT   FileName".**

<u>Prior to version 5.0</u>

D8   Record: KSS, ISS, JSS, CSS, ISSTYPE, [CSSMS(n), n=1, NCOMP]
          Format: 3I10, F10.0, I10, [free]
- This record is used to specify the point sources of specified concentrations. Note that those fluid sources included in the MODFLOW simulation but not specified herein are assumed to have zero concentration by default.

D8   Record: KSS, ISS, JSS, CSS, ISSTYPE, [CSSMS(n), n=1, NCOMP]
        Format: 3I10, F10.0, I10, [free]

- No changes in the meaning and number of the input variables as well as their input format; however, the range of allowed ISSTYPE codes has increased since the initial release of MT3DMS (see Table 5.1).

Since version 5.2, users can specify the input concentration of an injection well (ISSTYPE=2), i.e., CSS or CSSMS, as a negative integer code (IC). The absolute value of the integer code is the single cell location indicator of the extraction well whose output concentration is used as the input concentration for the injection well. For an extraction well located at layer K, row I, and column J, IC is computed as,

$$IC = NCOL \times NROW \times (K-1) + NCOL \times (I-1) + J .$$

where NCOL and NROW are the total numbers of columns and rows.

IV. CHANGES FOR THE RCT PACKAGE

Prior to version 5.1

   E1   Record: ISOTHM, IREACT, IRCTOP, IGETSC
         Format: 4I10
               • IREACT is an integer indicating the type of kinetic reaction simulated:
                 IREACT =0, no kinetic rate reaction is simulated;
                        =1, first-order irreversible reaction.

Changes since version 5.1

   E1   Record: ISOTHM, **IREACT,** IRCTOP, IGETSC
         Format: 4I10
               • IREACT is an integer indicating the type of kinetic reaction simulated:
                 IREACT =0, no kinetic rate reaction is simulated;
                        =1, first-order irreversible reaction;
                        =100, zeroth-order reaction (decay or production).

Prior to version 5.1

   E5   Array: RC1(NCOL, NROW)   (one array for each layer)
         Reader: RARRAY
               • RC1 is the first-order reaction rate coefficient for the dissolved (liquid)
                 phase (unit: T^{-1}). If a dual-domain system is simulated, the rate
                 coefficients for the liquid phase in the mobile and immobile domains are
                 assumed to be equal.

Changes since version 5.1

   E5   Array: RC1(NCOL, NROW)   (one array for each layer)
         Reader: RARRAY
               • If IREACT=1 (first-order kinetic reactions),
                 RC1 is the first-order rate coefficient for the dissolved (liquid) phase
                 (T^{-1}). If a dual-domain system is simulated, the rate coefficients for the
                 liquid phase in the mobile and immobile domains are assumed equal.
                 If IREACT=100 (zeroth-order decay or production),
                 RC1 is the zeroth-order reaction rate coefficient for the dissolved
                 (liquid) phase $(ML^{-3}T^{-1})$ (*positive for decay and negative for
                 production).* If a dual-domain system is simulated, the rate coefficients
                 for the liquid phase in the mobile and immobile domains are assumed
                 equal.

Prior to version 5.1

E6   Array: RC2(NCOL, NROW)   (one array for each layer)
      Reader: RARRAY
- RC2 is the first-order reaction rate coefficient for the sorbed (solid) phase (T^{-1}). If a dual-domain system is simulated, the rate coefficients for the sorbed phase in the mobile and immobile domains are assumed equal. Note that RC2 must be still specified although it is not used, if no sorption is included in the simulation.

Changes since version 5.1

E6   Array: RC2(NCOL, NROW)   (one array for each layer)
      Reader: RARRAY
- If IREACT=1 (first-order kinetic reactions),
RC2 is the first-order rate coefficient for the sorbed (solid) phase (T^{-1}). If a dual-domain system is simulated, the rate coefficients for the sorbed phase in the mobile and immobile domains are assumed equal.
If IREACT=100 (zeroth-order decay or production),
RC2 is the zeroth-order reaction rate coefficient for the sorbed (solid) phase ($MM^{-1}T^{-1}$) (*positive for decay and negative for production*). If a dual-domain system is simulated, the rate coefficients for the liquid phase in the mobile and immobile domains are assumed equal.