**Postprocessing relevant output of 1D-HYDRUS-MODFLOW to input of MT3DMS**

This document describes an automated postprocessing of the concentrations at the water table that are generated by the coupled 1D-HYDRUS-MODFLOW model. It generates input files for the recharge flux and concentration that is used by MT3DMS to simulate 3D transport in the saturated zone.

# Prerequisites

The coupled 1D-HYDRUS-MODFLOW needs to be set-up using a large number of stress periods. Only one set of water fluxes and input concentrations are provided to MT3DMS for each stress period. So even if the boundary condition remain constant during large part of the simulation, the user should define a large number of stress periods in order to pass a detailed breakthrough curve at the top of the water table to the transport model of MT3DMS.

Moreover the file with fluxes in the saturated domain with the extension “.ftl” is written in a formatted style.

# Running the tool

The postprocessing program is run by using an additional argument file: for example by typing

*<path>\postproces\_hydrus\_modflow2mt3dms.exe <argument\_file>*

on the command prompt line in the directory with the relevant files.

The argument file should contain:

* Line 1: the name of the zonation file
* Line 2: the name of the 1D-HYDRUS-MODFLOW output file with concentration data (by default named "Solute details")
* Line 3: the name of the 1D-HYDRUS-MODFLOW output file with water flow data (by default named "Sumvbot")
* Line 4: the horizontal model grid dimension of MODFLOW and MT3DMS (number of rows and number of columns)
* Line 5: the root of the files to be created with recharge concentration for each stress period; input for MT3DMS
* Line 6: the format of the concentration in the files to be created with recharge concentration for each stress period
* Line 7: 1D-HYDRUS-MODFLOW output file with water fluxes in saturated part
* Line 8: file to be created with water fluxes in saturated part with recharge; input for MT3DMS
* Line 9: horizontal surface area of model cells; Unit: the square of the unit of length used in MT3DMS domain.

An example is given in Figure 1.

"ex.zon" zonation file

"Solute details" 1D-HYDRUS-MODFLOW output file with concentration data at the water table interface

"Sumvbot" 1D-HYDRUS-MODFLOW output file with water flow data at the water table interface

26 18 number of columns, number of row in the saturated model grid

"ex.crch" root of the files to be created with 'recharge' concentration; is iput for MT3DMS

(26F12.4) format of output of 'recharge'concentration

"ex.ftl" 1D-HYDRUS-MODFLOW output file with water fluxes in saturated part

"ex.ftl2" file to be created with water fluxes in saturated part with recharge; input for MT3dMS

0.04 horizontal surface area of model cells; Unit: the square of the unit of length used in MT3DMS domain

Figure 1 Example of the argument file

# Relevant input files

The postprocessing program uses 4 files from the coupled 1D-HYDRUS-MODFLOW model as input:

1. The zonation file
2. The output file “Solute Details”
3. The output file “Sumvbot”
4. The outputfile with the water fluxes in the saturated part of the domain

## 1 The zonation file

This file connects the profiles of the 1D HYDRUS models to the 2D horizontal grid of MODFLOW and MT3DMS. It is also an input file for the coupled 1D-HYDRUS-MODFLOW model. An example of this file is given in Figure 2.

1 # Number of zone arrays

ZONE1 # name of zone array

INTERNAL 1 (3I2) 1 # header line of zone array

2 2 2 # array row 1

2 1 2 # array row 2

2 2 2 # array row 3

Figure 2 Example of zonation file

The postprocessing program assumes this file only contains 1 zone of arrays, see line 1 of the example. It also assumes that in line 3 the INTERNAL input option is used and the zonation arrays are given from line 4 onwards using the format given in line 3 [(3I2) in this example].

## *2* The output file “Solute Details”

This file contains output of the coupled 1D-HYDRUS-MODFLOW model, in especially the solute concentration at the water table for all profiles that are calculated by the Hydrus 1D model. An example is shown in Figure 3. The filename that is automatically given by the 1D-HYDRUS-MODFLOW model is “Solute details”.

Profile NO: Time Conc\_WT Conc\_flux Time step Stress period

[-] [T] [M/L3] [M/L2/T] [-] [-]

1 1.00 0.000E+00 0.000E+00 1 1

2 1.00 0.000E+00 0.000E+00 1 1

1 2.00 0.000E+00 0.000E+00 1 2

2 2.00 0.000E+00 0.000E+00 1 2

1 3.00 0.000E+00 0.000E+00 1 3

2 3.00 0.000E+00 0.000E+00 1 3

……

……

1 1528.00 0.779E+01 -0.383E-02 1 1528

2 1528.00 0.000E+00 0.000E+00 1 1528

1 1529.00 0.773E+01 -0.380E-02 1 1529

2 1529.00 0.000E+00 0.000E+00 1 1529

1 1530.00 0.768E+01 -0.377E-02 1 1530

2 1530.00 0.000E+00 0.000E+00 1 1530

……

……

Figure 3 Example of the solution detail output file

From this file, the profile number and the concentration at the water table are read. For each time step the concentration of the profile are mapped on the horizontal model grid of MT3DMS using the zonation array and written to different files that can be used as input files for MT3DMS.

## 3 The output file “Sumvbot”

From this file the water fluxes at the bottom boundaries of the 1D-HYDRUS columns are read. This file contains water fluxes at all internal calculation time steps of the Hydrus part of the model. The postprocessing tools automatically obtains the value at the end of each stress period out of these series for all 1D-HYDRUS columns by analysing the first column with cumulative time data. An example of the file is given in Figure 4.

T= 1.00000000E-03 DT= 1.00000000E-03 VBOT= -1.25687928E+00 SUMV= -1.25687928E-03 Begin of stress period 1 for HYDRUS column 1

T= 2.00000000E-03 DT= 1.00000000E-03 VBOT= -1.09542209E+00 SUMV= -2.35230137E-03

…………..

T= 9.74417419E-01 DT= 1.00000000E-01 VBOT= -3.09168892E-03 SUMV= -2.58258697E-02

T= 1.00000000E+00 DT= 2.55825807E-02 VBOT= -2.98185030E-03 SUMV= -2.59021532E-02 End of stress period 1 for HYDRUS column 1

T= 1.00000000E-03 DT= 1.00000000E-03 VBOT= -1.25687928E+00 SUMV= -1.25687928E-03 Begin of stress period 1 for HYDRUS column 2

T= 2.00000000E-03 DT= 1.00000000E-03 VBOT= -1.09542209E+00 SUMV= -2.35230137E-03

T= 3.29947917E-03 DT= 1.29947917E-03 VBOT= -9.35986691E-01 SUMV= -3.56859657E-03

…..

T= 9.74417419E-01 DT= 1.00000000E-01 VBOT= -3.02884688E-03 SUMV= -2.58050665E-02

T= 1.00000000E+00 DT= 2.55825807E-02 VBOT= -2.92049567E-03 SUMV= -2.58797803E-02 End of stress period 1 for HYDRUS column 2

T= 1.02558258E+00 DT= 2.55825807E-02 VBOT= 2.05085775E-03 SUMV= 5.24662341E-05 Begin of stress period 2 for HYDRUS column 1

T= 1.12302432E+00 DT= 9.74417419E-02 VBOT= 2.87339001E-03 SUMV= 3.32454362E-04

…

T= 1.90255826E+00 DT= 9.74417419E-02 VBOT= -8.11766727E-04 SUMV= 1.00218596E-05

T= 2.00000000E+00 DT= 9.74417419E-02 VBOT= -7.91587707E-04 SUMV= -6.71118254E-05 End of stress period 2 for HYDRUS column 1

T= 1.02558258E+00 DT= 2.55825807E-02 VBOT= 2.93068788E-03 SUMV= 7.49745593E-05 Begin of stress period 2 for HYDRUS column 2

…..

T= 1.90255826E+00 DT= 9.74417419E-02 VBOT= -7.70616111E-04 SUMV= 1.79835847E-04

T= 2.00000000E+00 DT= 9.74417419E-02 VBOT= -7.55304682E-04 SUMV= 1.06237643E-04 End of stress period 2 for HYDRUS column 2

……..

Figure 4 Example of output file “SumvBot”

## 4 The output file with the water fluxes in the saturated part of the domain

This large file contains all water fluxes that are calculated between the model nodes as well as the boundary fluxes in the saturated part of the model domain for all stress periods. This file is equal to a standard output file of MODFLOW, with the exception that input flux from the groundwater recharge. The recharge fluxes must be added at specific location for each time step. That is arranged in the postprocessing tool.

# Output files

Two type of output files are created by the program. The first set contains the recharge concentration in the upper layer of the MT3DMS model grid for a single time step. The timestep number is added to the root name that was given in the argument file. For the example the files ex.crch1, ex.crch2 , ex.crch3 and so on are created.

The second type of output is the adapted flux file. The name of this file was given in the argument file. This file now also contains recharge fluxes for all time steps.

# Link with in the MT3dMS input files

The MT3DMS input files need to contain information of the link to the output files that are created by the postprocessing program. This is arranged in the following input files:

1. The MT3DMS name file
2. The sink source file

## 1 The MT3DMS name file

The MT3DMS name file must contain the links to all data files with the recharge concentration arrays for all time steps using the standard convention of the MT3DMS name file: by using:

(1) the keyword “DATA”,

(2) a unique unit number and

(3) the data file name for each data file.

An example of the extension for 2 timesteps is shown in Figure 5.

…

data 90 ex.crch1

data 91 ex.crch2

….

Figure 5 Example of additional input in the MT3DMS name file

## 2 The sink source file

In the sink source input file of MT3DMS, the recharge concentration can now be linked with the external files using the unit numbers that are given in the MT3DMS name file. The format of the arrays should be equal to the format specified in the argument file.

An example is shown in Figure 6.

F F T F F F FWEL,FDRN,FRCH,FEVT,FRIV,FGHB

1000 MXSS

1 INRCH (time step 1)

90 1.0 (26F12.4) -1 CRCH (time step 1)

0 NSS (time step 1)

1 INRCH (time step 2)

91 1.0 (26F12.4) -1 CRCH (time step 2)

0 NSS (time step 2)

Figure 6 Example of a sink source file with a link to the external recharge concentration files

In this example, the recharge concentration of time step 1 and 2 are linked to the file connected to unit number 90 and 91 respectively (defined in the example MT3DMS name file, in Figure 5). The format (26F12.4) is equal to the format in the example of the argument file (Figure 1).

A more detailed description of the MT3DMS input files is given in the MT3DMS manual.