

MODFLOW Data Extractor Program

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Preface

This report describes a post-processing program for *MODFLOW* and *MODFLOW-GWT*, three-dimensional ground-water flow and solute-transport models developed by the U.S. Geological Survey (USGS). The new program facilitates data analysis of model results by extracting subsets of data from complex three-dimensional simulation output files.

The code and documentation for this software, called *EXTRACTOR*, are available for downloading over the Internet from a USGS software repository. The repository is accessible from links on a Web site for USGS ground-water models at <u>http://water.usgs.gov/nrp/gwsoftware/</u> or <u>http://water.usgs.gov/software/ground water.html</u>. When this code is revised or updated in the future, new versions or releases will be made available for downloading from this same site.

Although extensive testing of the code indicates that it will yield reliable output for a variety of problems, future applications might reveal errors that were not detected in the test cases. Users are requested to notify the USGS of any errors found in this documentation or the computer program by using the contact information shown on the distribution Web site.

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Abstract

EXTRACTOR is a program that extracts data from formatted and labeled *MODFLOW* head or drawdown files or from *MODFLOW-GWT* concentration or velocity files. The user specifies the number of rows, columns, and layers in the target data file, the desired time step or move number, and the range of rows, columns, and layers for which data should be extracted and written to a new text file. The new text file can then be imported into other data-analysis programs.

Introduction

MODFLOW-2000 is a three-dimensional ground-water-flow model (Harbaugh and others, 2000). Output files from *MODFLOW* and related programs, such as *MODFLOW-GWT* (Konikow and others, 1996), are often written as large arrays (or matrices) of three-dimensional spatial data at multiple time levels. Users may want to analyze just small parts or subsets of the total data set, but this is difficult with the standard output format. For example, from the calculated three-dimensional head distribution, the user may want to view or contour heads in a particular cross section, or may wish to view or plot a single vertical line of concentrations corresponding to the location of a well in a transport simulation. There is no simple and general way to remove these data from the output files, other than manually going through the data, pulling out numbers, and copying them into a spreadsheet or other program. *MODFLOW* and *MODFLOW-GWT* simulation results can also be difficult to import directly into other data-analysis programs because of the idiosyncratic structure of the output files.

A new computer program, called *EXTRACTOR*, has been developed as post-processing software to help lessen these limitations. *EXTRACTOR* is a program that extracts data from formatted (text) and labeled *MODFLOW* head or drawdown files and from *MODFLOW-GWT* concentration or velocity files. It reads one of the compatible model output files and allows the user to select points, lines, planes, or three-dimensional blocks of data. The selected data are written to a new text file, which can then be imported into other data-analysis programs. This report documents and describes the use of the *EXTRACTOR* program.

Computer Code

The computer code is written in Fortran, using standard Fortran-90 conventions. It reads *MODFLOW* and *MODFLOW-GWT* output files that have been written as text files. In *MODFLOW* output conventions, such files are called "formatted" files (see Harbaugh and others, 2000, p. 52-54). *MODFLOW* output files can also include header lines before each block of data. These header lines describe the location and time step for which the block of data was written. In *MODFLOW* terminology, such files are defined as "labeled." *MODFLOW-GWT* output files include labeled header lines by default.

Instructions

Required Files

In order to run the EXTRACTOR program, the following files are needed:

- 1. The executable file, *EXTRACTOR.EXE*.
- 2. An input file. This file is a text file that tells *EXTRACTOR* the nature of the data set and which data points are to be extracted. Instructions for how to create this file follow in the "Input File" section. Note that different data file types require different input files. The name of this file will be included in the name of the output file generated by *EXTRACTOR* (see "Output File" section below).
- 3. At least one data file. This is the file on which the *EXTRACTOR* program will operate, and it is usually generated as output from either a *MODFLOW* or *MODFLOW-GWT* simulation. Note that more than one data file can be present in the same directory; the user will specify which file is to be used when the program is run.

Input File

The user should first scan the data file and determine the size of the data sets (number of columns, rows, and layers) and confirm that data for the desired time period are contained in the file to be read.

Next, the user must create an input file that tells *EXTRACTOR* about the data to be read and what data to extract and save. To accomplish this task, create a text file using a text editor or word-processing software (but make sure it is saved as text only).

The input file will always consist of six lines (or records). All input variables are read using free formats. In free format, variables are separated by one or more spaces or by a comma and optionally one or more spaces. Blank spaces are not read as zeros. Detailed input instructions follow; variables that are optional are enclosed in brackets, as in {option}.

FOR EACH SIMULATION:

1. Data: FTYPE

FTYPE The file type, which should be one of the following character strings:

HEAD	indicates a MODFLOW head file will be read.
DRAW	indicates a MODFLOW drawdown file will be read.
CONC	indicates a <i>MODFLOW-GWT</i> concentration file will be read.
VELO	indicates a MODFLOW-GWT velocity file will be read.

Notes:

Any file to be read by the *EXTRACTOR* program must be a formatted (ASCII text) and labeled file created by *MODFLOW* or *MODFLOW-GWT*. *EXTRACTOR* will not read binary files. Concentration and velocity output files created by *MODFLOW-GWT* automatically include labels if they are formatted text files. *MODFLOW-GWT* has an option to write a separate concentration output file either as a matrix or as a table of values; *EXTRACTOR* will read only the matrix style and is not compatible with the table style.

2. Data: NCOL NROW NLAY

NCOL	Total number of columns of data in the output file.
NROW	Total number of rows of data in the output file.
NLAY	Total number of layers of data in the output file.

Notes:

These three values describe the total number of columns, rows, and layers of data in the file to be read, where the columns, rows, and layers refer to the *MODFLOW* or *MODFLOW-GWT* simulation grid. If a transport subgrid is used to simulate solute transport, then for FTYPE CONC and VELO, the number of columns, rows, and layers in Record 2 correspond with the respective values for the transport subgrid, which may be less than that used in the primary MODFLOW grid for simulating flow.

	3.	Data:	NPER	NTSTEP	{IMOV}
NPER The number of the stress period for which data are to be extracted.			iod for which data are to be extracted.		
NTSTEP		EP	The number of the time step for which data are to be extracted.		
IMOV The number of the transport time increment for which data are to be extr			time increment for which data are to be extracted.		
Only specify this parameter for FTYPE = CONC.			for $FTYPE = CONC$.		

Notes:

Data may be extracted for only one time step in any given run of *EXTRACTOR*. These variables are expressed as integer numbers. So, for example, if head data were to be extracted from Time Step 4 of Stress Period 2, Record 3 would read "4 2".

4. Data: COL1 COLEND

COL1 The column number of the first column in the range of data to be extracted. The column number of the last column in the range of data to be extracted. COLEND

Notes:

COLEND must be greater than or equal to COL1 and less than or equal to NCOL.

ROW1 ROWEND 5. Data:

ROW1 The row number of the first row in the range of data to be extracted. The row number of the last row in the range of data to be extracted. ROWEND

Notes:

ROWEND must be greater than or equal to ROW1 and less than or equal to NROW.

6. Data: LAY1 LAYEND

LAY1 The layer number of the first layer in the range of data to be extracted. The layer number of the last layer in the range of data to be extracted.

Notes:

LAYEND

LAYEND must be greater than or equal to LAY1 and less than or equal to NLAY.

Output File

Running *EXTRACTOR.EXE* will create a new text file named *CUT.inputname*, where *inputname* is the name of the input file containing the input data for *EXTRACTOR* (as described in the previous "Input File" section). This new file contains a sequential list of data values for the desired subset of the original data file, arranged in standard *MODFLOW* style with column-row arrays listed for each layer in sequence, with some differences depending on the dimensionality of the data (see the "Output File Examples" section for details, including exceptions to the standard formatting).

The dimensionality of the extracted data set will be controlled by the values of COL1, COLEND, ROW1, ROWEND, LAY1, and LAYEND. If COL1 = COLEND, ROW1 = ROWEND, and LAY1 = LAYEND, a single point of data located at (COL1, ROW1, LAY1) will be extracted. If one of the three directions has unequal values, a one-dimensional data set (that is, a line) will be extracted. If two of the directions are different, a plane will be extracted. If all three are different, a three-dimensional data set will be extracted.

The format of the written data will depend on the type of file that was manipulated. Labeled head and drawdown files contain a format specification in the header line. In this case, the format specification is read by the *EXTRACTOR* program and the same format is used when writing the extracted data to the new output file. *MODFLOW-GWT* output files for concentration and velocity matrices are always written using a format of (1P10E12.4), and *EXTRACTOR* will write the extracted data for concentration and velocity using the same format specification.

If a scalar data type was extracted (head, concentration, or drawdown), the files will be written according to standard *MODFLOW* conventions for writing two-dimensional arrays of row and column data in blocks for each layer. See the "Output File Examples" section for details.

MODFLOW-GWT velocity output files contain three values for every node—the velocity in the column direction, in the row direction, and in the layer direction, in that order, grouped by layer. That is, for each given time level, this file includes all the values for velocity in the column direction for the first layer, then all values for velocity in the row direction for the first layer, followed by all values for velocity in the layer direction for the first layer, then repeats that sequence for all the remaining layers until all data for that time level are written. This sequence is then repeated for each additional time level (if there are any). *EXTRACTOR* will write the extracted velocity data in a modified style that should be more compatible with commercial plotting or contouring packages. *EXTRACTOR* will first write all columns, rows, and layers of the extracted data for velocity in the column direction, then all columns, rows, and layers for velocities in the row direction, followed by all columns, rows, and layers for velocity in the layer direction conventions. See the "Output File Examples" section for an example of this format.

Output files generated by EXTRACTOR do not include any header lines or labels.

Input File Examples

Head:

Following is an example of an *EXTRACTOR* input file designed to operate on a *MODFLOW* head file. A *MODFLOW* simulation was run using a grid that was 40 columns long, 20 rows wide, and 10 layers deep, and we wish to extract data over the full depth of the system, but only from columns 15 to 25 and from rows 5 to 15 (perhaps the area around a pumping well, for example). A transient flow simulation was run for one stress period containing ten time steps, and we wish to isolate the head values at the end of time step 3. An input file to extract these data would read as follows:

HEAD	FTYPE	
40 20 10	NCOL NROW NLAY	
1 3	NPER NSTEP	
15 25	COL1 COLEND	
5 15	ROW1 ROWEND	
1 10	LAY1 LAYEND	
	1	

The name of the head file to be read will be specified when *EXTRACTOR* is run (see "Running *EXTRACTOR.EXE*" below).

Concentration:

Concentration extraction input files follow a similar structure to head input files. Because time-step increments used to solve the solute-transport equation can be smaller than the time steps used to solve the flow equation, *MODFLOW-GWT* can also record concentrations at specified particle move intervals (or transport time increments) in addition to recording concentration values at specific stress periods and time steps. Therefore, for a concentration file the user must specify the move number (IMOV or transport time increment number) on line 3 of the input data file. IMOV must always be specified for a concentration file. Values of IMOV can be found both in the header lines of the separate concentration file or in the output (listing) file for the GWT Process of *MODFLOW*.

Following is an example of an *EXTRACTOR* input file designed to operate on a *MODFLOW-GWT* concentration file. For the example used above for the head extraction file, transport was simulated simultaneously with flow and we wish to examine concentrations along a vertical line where a fully penetrating well is located (row 10, column 20, all layers). We are interested in concentration values at the 250^{th} transport time increment (IMOV = 250) in the third time step of the first stress period. The corresponding input file would be:

CONC	FTYPE
40 20 10	NCOL NROW NLAY
1 3 250	NPER NSTEP IMOV
20 20	COL1 COLEND
10 10	ROW1 ROWEND
1 10	LAY1 LAYEND

Running EXTRACTOR.EXE

After setting up an *EXTRACTOR* input file, the program is ready to run. To start it, doubleclick on the executable file (*EXTRACTOR.EXE*). This action will open a new window and bring up a dialog that asks:

Enter the name of the "EXTRACTOR" INPUT DATA FILE:

Type in the name of the data input file that you have created and hit return (this file can be named "myinput.txt" or something similar). You are then prompted with:

Enter the name of the FTYPE DATA FILE:

where *FTYPE* is the type of file specified in the input data file. Type in the name of the *MODFLOW* or *MODFLOW-GWT* output data file to be read. Hit return.

The program will then execute and, if it terminates normally, create and write an output file according to the desired specifications. The name of the new output file depends on the name of the input file. For example, if "myinput.txt" is the name of the *EXTRACTOR* input file, the program will automatically assign the name "CUT.myinput.txt" to the output file from *EXTRACTOR*.

The data in the *EXTRACTOR* output file should be easy to import into graphical post-processing software programs.

Output File Examples

Scalar:

Scalar data sets (head, concentration, and drawdown) are written in standard *MODFLOW* format. If *EXTRACTOR* was run on a head data set and extracted columns 4 through 7, rows 2 through 4, and layers 5 and 6, the output would be written as:

[Written in the form FTYPE(COLUMN #, ROW #, LAYER #)]

HEAD(4,2,5)	HEAD(5,2,5)	HEAD(6,2,5)	HEAD(7,2,5)
HEAD(4,3,5)	HEAD(5,3,5)	HEAD(6,3,5)	HEAD(7,3,5)
HEAD(4,4,5)	HEAD(5,4,5)	HEAD(6,4,5)	HEAD(7,4,5)
HEAD(4,2,6)	HEAD(5,2,6)	HEAD(6,2,6)	HEAD(7,2,6)
HEAD(4,3,6)	HEAD(5,3,6)	HEAD(6,3,6)	HEAD(7,3,6)
HEAD(4,4,6)	HEAD(5,4,6)	HEAD(6,4,6)	HEAD(7,4,6)

Remember that the actual format of the output numbers, including the number of significant figures, will be controlled by the format of original data set (in the case of head and drawdown files, this format is a controllable option in *MODFLOW*, whereas in the case of concentration or velocity files, data are automatically assigned (1P10E12.4) format).

Vector:

Velocity data are vectors with three components—velocity in the column direction (termed VELCOL in this example), row direction (VELROW), and layer direction (VELLAY). If *EXTRACTOR* was run on a velocity data set in which columns 8 through 10, rows 1 and 2, and layers 5 and 6 were extracted, the output file would be written as:

```
VELCOL(8,1,5) VELCOL(9,1,5) VELCOL(10,1,5)
VELCOL(8,2,5) VELCOL(9,2,5) VELCOL(10,2,5)
VELCOL(8,1,6) VELCOL(9,1,6) VELCOL(10,1,6)
VELCOL(8,2,6) VELCOL(9,2,6) VELCOL(10,2,6)
```

VELROW(8, 1, 5)VELROW(9,1,5) VELROW(10,1,5) VELROW(8, 2, 5)VELROW(9,2,5)VELROW(10,2,5) VELROW(8,1,6) VELROW(9,1,6)VELROW(10,1,6) VELROW(8,2,6) VELROW(9,2,6)VELROW(10,2,6) VELLAY(8,1,5) VELLAY(9,1,5)VELLAY(10,1,5) VELLAY(8,2,5) VELLAY(9,2,5)VELLAY(10,2,5) VELLAY(8,1,6)VELLAY(9,1,6)VELLAY(10,1,6) VELLAY(8,2,6) VELLAY(9,2,6) VELLAY(10,2,6)

Exception:

There is one exception to the above formatting—if a two-dimensional data set (that is, a plane) with changing indices in the row and layer directions is extracted, the rows will be arranged in the ways columns are in a standard format. For example, going back to the previous HEAD output file example, this time with only column 4 extracted, the output would be written as:

HEAD(4,2,5) HEAD(4,3,5) HEAD(4,2,6) HEAD(4,3,6)

Summary

A new program, named *EXTRACTOR*, has been written to help in the post-processing of data sets produced by *MODFLOW* and *MODFLOW-GWT* simulation programs. It enables the isolation of a limited subset of data from a large three-dimensional data set. This program capability can facilitate, for example, contouring of values in any two-dimensional plane or cross section of interest in a complex three-dimensional data set.

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