Program Developments for Modeling Groundwater Flow in Three-Dimensional Heterogeneous Aquifers with MODFLOW and MODFLOWP

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PREFACE

This report documents utility code developments and modifications for MODFLOW and MODFLOWP which provide new model set-up, performance monitoring and output capabilities. Source code for these modifications is available under the listing for this report through the home page of the Center for Geophysical Investigation of the Shallow Subsurface at http://kihei.idbsu.edu/cgiss_pub.html. This report, including the modified MODFLOW and MODFLOWP codes, are public domain and as such may be used and copied freely. The developed programs have been tested. However, no warranty is given that the code is completely error-free. No liability is assumed for any damage or loss that may result from use of our programs. If you do encounter problems with the code, find errors, or have suggestions for improvement, please contact one of the authors at the addresses below.

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ABSTRACT

This report documents (1) a number of stand-alone utilities to assist with input to MODFLOW and (2) code modifications internal to MODFLOW and MODFLOWP. These were developed to improve ease of use of MODFLOW and MODFLOWP for modeling groundwater flow in three-dimensional heterogeneous systems. Several utilities to assist with input to MODFLOW are specifically designed for use with the Groundwater Modeling System (GMS) pre- and post-processor package.

New features for MODFLOW include routines for: (1) assignment of material blocks and material types to these blocks within a given three-dimensional grid mesh; (2) generation of the Block Centered Flow (BCF) file for heterogeneous aquifers with material properties assigned to blocks, and with internal calculation of leakance and thickness-factored parameters (T, S); (3) distribution of pumping rate for individual model layers for a well that draws from or injects into multiple layers; (4) calculation of weighted drawdown for an observation well screened over multiple layers; and (5) customizing the drawdown output file to contain data for a specified number of observation wells, rather than every node in the domain.

For MODFLOWP, the program has been modified to: (1) simplify input by making the .PAR file free format; (2) allow the user to easily change the number and combination of parameters for estimation in a given run by modifying one line rather than regenerating the .PAR file; (3) automatically calculate ROFFs, COFFs, and TOFFs for observation wells; (4) notify the user during program execution when lower or upper parameter ranges are exceeded; and (5) provide monitoring of run time.

TABLE OF CONTENTS

LIST OF FIGURES

Page

LIST OF EXAMPLE FILES

Example File Page

1. INTRODUCTION

MODFLOW (McDonald and Harbaugh, 1988) is perhaps the most widely-used numerical code for groundwater modeling due to its ability to handle complex groundwater flow situations, including three-dimensional irregular solution domains, heterogeneous aquifers, and a comprehensive range of boundary conditions and flow processes. It has been thoroughly tested against analytical solutions and has been used for a wide variety of field applications. An inversion code based on MODFLOW, MODFLOWP (Hill, 1992), provides automated estimation of hydrologic parameters. We have been using both MODFLOW and MODFLOWP in our modeling of pumping tests in a shallow alluvial aquifer where both pumping and observation wells are partially penetrating wells over different depth intervals in the aquifer. Modeling of these tests requires a three-dimensional distribution of aquifer parameters to achieve matches with observed behavior (Barrash et al., 1995; 1997).

This report is an outgrowth of these efforts to model heterogeneous three-dimensional systems and presents a number of utilities and code modifications to expedite use of MODFLOW (Section 2) and MODFLOWP (Section 3) by improving input and output ease and flexibility. For MODFLOW, some of these utilities are designed to operate in conjunction with the Department of Defense Groundwater Modeling System (GMS), a comprehensive pre- and post-processing software package for MODFLOW, as well as other common groundwater modeling codes.

In particular, this report presents utilities to address the following input and output issues associated with three-dimensional systems and pumping test applications of MODFLOW: (1) assignment of material blocks and material types to these blocks within a given grid mesh; (2) generation of the Block Centered Flow (BCF) file for heterogeneous aquifers with material properties assigned to blocks and internal calculation of leakance and thickness-factored parameters (T, S); (3) distribution of pumping rate for individual model layers for a well that draws from or injects into multiple layers; (4) calculation of weighted drawdown for an observation well screened over multiple layers; and (5) creation of a drawdown output file to contain data for only a specified number of observation wells rather than for every node in the model.

For MODFLOWP, the program has been modified to: (1) simplify input by making the .PAR file free format; (2) allow the user to easily change the number and combination of parameters for estimation in a given run by modifying one line rather than regenerating the whole .PAR file; (3) automatically calculate ROFFs, COFFs, and TOFFs; (4) notify the user when parameter values go beyond upper and lower limits for parameters during estimation runs; and (5) monitor run time.

2. UTILITIES FOR USE WITH MODFLOW

2.1 Automatic Generation of Grid Cells and Assignment of Cell Properties

2.1.1. Problem

Many natural geologic materials are heterogeneous. Accurately characterizing the spatial distribution of hydraulic properties may be the most critical step in modeling groundwater flow

and transport in strongly heterogeneous aquifers. A heterogeneous aquifer commonly is characterized by dividing the aquifer into many material blocks or zones, each of which is assumed to be homogeneous (i.e., to have constant hydraulic properties associated with the geologic material within each block or zone).

GMS defines a block (3D) or zone (2D) by selecting a group of cells, and it then assigns a material type, MATID, to the block or zone according to user-provided information. (NOTE: for brevity in this report we will henceforth refer only to blocks) This procedure is applied to define all blocks in the solution domain. Hydraulic properties of each grid cell are then identified through the MATID. In practice this procedure can be very time-consuming and error-prone, especially when the model structure is highly heterogeneous.

Not only must three-dimensional grids be generated before the material blocks can be defined, but commonly the model is modified after initial runs such that the grid must be changed, and/or the geometry or distribution of blocks are changed. As a result, previously defined material blocks are no longer useful because the associated cells have been changed. Hence, the material blocks have to be redefined for each new discretization. Without a utility to automate this process, significant amounts of time are needed to generate each new or modified model structure, introducing the potential for errors to be incorporated.

2.1.2. Solution

We have developed the program BLOCK.FOR to accurately define the material blocks and assign the MATIDs for all cells. Whenever the spatial discretization is changed, new MATIDs can be obtained by running the BLOCK.FOR program. The BLOCK.FOR program is a stand-alone utility for use with GMS as a pre-processor to generate the three-dimensional grid file (*filename*.3DG).

BLOCK.FOR works in the following way. Assume the solution domain is a volume consisting of NLAY model layers, each of which has NCOL columns and NROW rows. Coordinates of the columns and rows are defined by X(i), i = 1,...,NCOL+1 and Y(j), j = 1,...,NROW+1, respectively (Figure 1). Also assume that each model layer (not necessarily the same as a geologic or hydrostratigraphic layer) includes several types of materials, and each material has a different set of hydraulic properties that is constant for that type of material. On a model-layer by model-layer basis, BLOCK.FOR reads information on the number and locations of blocks and the material types associated with the blocks. To reduce the input effort, the user assigns a background MATID for each layer, which usually would be the material type that is most abundant in a given layer. Thus, the user need only define the specific block geometry and MATIDs for the remaining portions of a given layer.

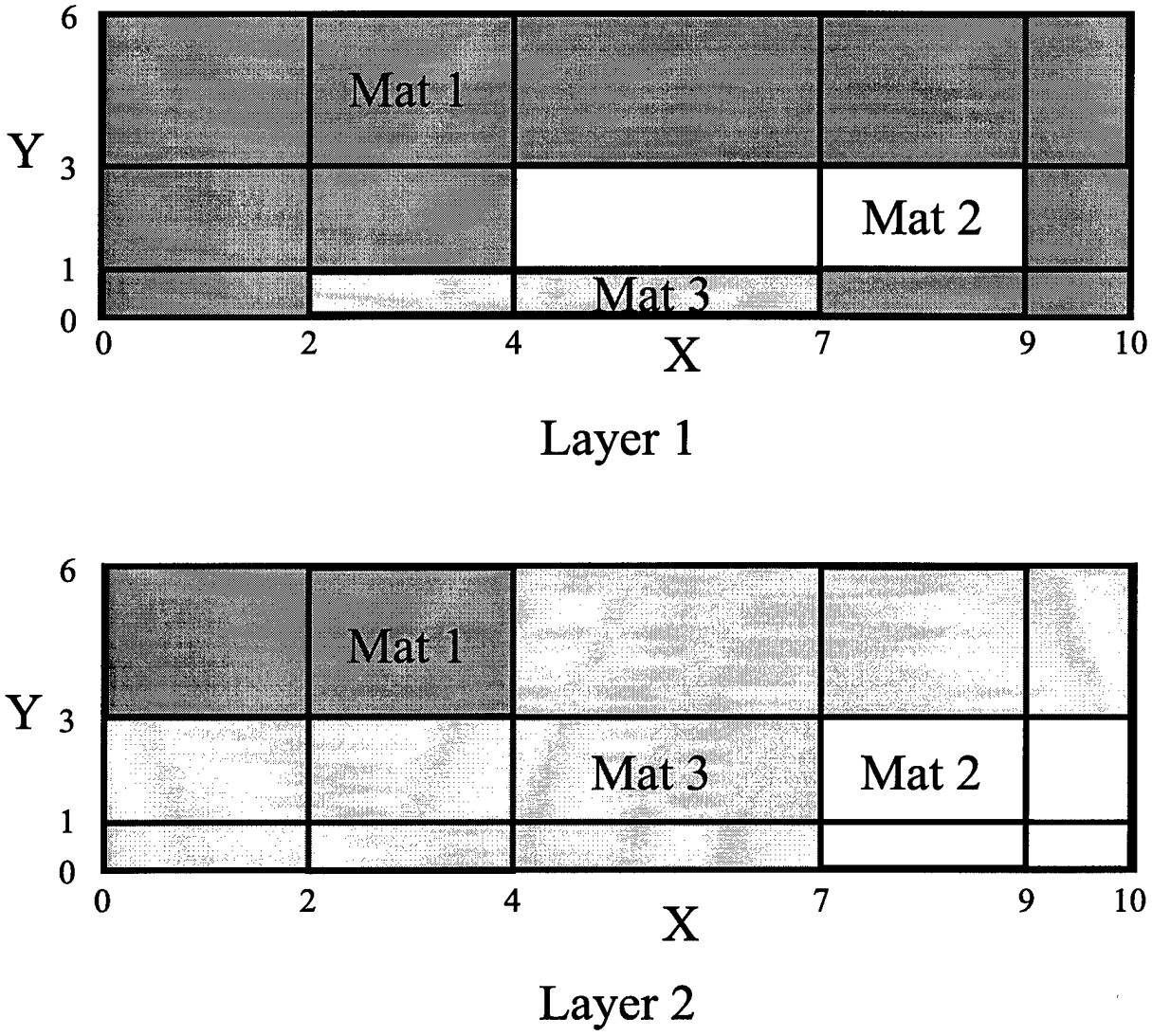


Figure 1. Plan view of material blocks described in the example application (Section 2.1.4). Layer 1 is at the top and Layer 2 is at the bottom.

In plan view each block, *k*, in a given layer (i.e., *k* = 1 to NBLOCK, or total number of blocks in a given layer) is a rectangular area that is uniquely defined by the coordinates of its lower left corner (XLL(*k*),YLL(*k*)) and upper right corner (XUR(*k*),YUR(*k*)). The hydraulic properties of each block are identified by its material type, MATID(k). With this information, the aquifer system heterogeneity can be built into the model using BLOCK.FOR.

2.1.3. Input Instructions for the BLOCK.FOR program

The BLOCK.FOR program requires two input files: BLOCK.IN and a .3DG file. These files are described below with examples.

2.1.3.1. BLOCK.IN

The BLOCK.IN file defines the geometry and MATID of each block and gives the background material type for each layer. Thus, there are NLAY data sets in BLOCK.IN, one for each layer, m (i.e., m = 1 to NLAY). Inputs for each layer are:

1. MATID(m), NBLOCK(m)

Background material type and number of blocks for layer m. A line then follows for each block, k (k = 1 to NBLOCK(m)), in layer m:

2. MATID(k), XLL(k), YLL(k), XUR(k), YUR(k)

Material type and coordinates of the lower left (LL) and upper right (UR) corners of block k. If this layer is homogeneous then NBLOCK(m) = 0. Inactive blocks have MATID(k) = 0. It is important that the defined blocks in a layer should not overlap, although they will have corners and sides in common with adjacent blocks.

2.1.3.2. .3DG File

The .3DG file defines the solution domain and its discretization. It contains the following information:

1. NLAY, NCOL, NROW	Numbers of layers, columns, and rows
2. X(i), i = 1, NCOL+1	X coordinates of nodes in a layer
3. Y(j), j = 1, NROW+1	Y coordinates of nodes in a layer

A .3DG file can be obtained directly from GMS in the following way: when a solution domain has been defined in GMS (i.e., the grid has been formed), save the grid information in a file using the GMS command sequence: **File---> Save** and provide a filename to go with the filespec of .3DG. The BLOCK.FOR program modifies this file and then uses the same filename for the output file, overwriting the original file. This modified new *filename*.3DG file has MATID information for each cell - which is what is needed by GMS to generate the model structure (i.e., distribution of materials in a given three-dimensional grid). Then, using BCF_IN.FOR the *filename*.3DG file can be used to generate the BCF file needed by MODFLOW (section 2.2). Once the new *filename*.3DG file is generated, it remains valid even if the horizontal discretization of the grid is changed as long as the following have not changed: (1) the overall model dimensions, (2) the number and dimensions of layers, and (3) the locations of blocks.

2.1.4. Example Application

This example shows how the BLOCK.FOR program works. The input and output files for the example are also illustrated. First, assume a region of an aquifer (surface area of 10 x 6 length units^2) is discretized into blocks bounded in the x direction at 0, 2, 4, 7, 9, and 10 length

units, and in the y direction at 0, 1, 3, and 6 length units. The model of the aquifer has two layers: the upper layer is 5 units thick and the lower layer is 10 units thick (Figure 1). Three materials (MATID 1, 2, and 3) are identified and their distributions in each layer are shown in Figure 1. In layer 1, the most prevalent material (i.e., background material) is MATID1. There are two blocks defined in layer 1: one consists of MATID2 and is defined by its lower left corner (4, 1) and upper right corner (9, 3); the other block consists of MATID3 and is defined by lower left corner (2, 0) and upper right corner (7, 1). In layer 2, the background material is MATID3 and there are two material blocks as in layer 1: a block with MATID1 defined by lower left corner (0, 3) and upper right corner (4, 6); and a block with MATID2 defined by lower left corner (7, 0) and upper right corner (10, 3).

It should be noted that, the convention used here for locating blocks has the origin in the lower left-hand corner of a layer when viewing the layer in plan view. However, the default origin used by GMS is located at (100, 250, -10) for the example of Figure 1 and Example Files 1 and 2. It should be noted that the internal GMS coordinate system can be specified by the modeler such that it agrees with the BLOCK.FOR routine.

Example File 1. Example BLOCK.IN file

BLOCK.IN Explanation

```
1 2              1=MATID1 for background; 2=two blocks will be defined in following lines
2 4. 1. 9. 3.    2=MATID2, lower left (4,1) and upper right (9,3) corners
3 2. 0. 7. 1.    3=MATID3, lower left (2,0) and upper right (7,1) corners
3 2              3=MATID3 for background, 2=two blocks will be defined in following lines
1 0. 3. 4. 6.    1=MATID1, lower left (0,3) and upper right (4,6) corners
2 7. 0. 10. 3.   2=MATID2, lower left (7,0) and upper right (10,3) corners
```

Below is an example .3DG file generated when a model grid is defined in GMS, and in which MATIDs are not yet defined. This file is used for input to BLOCK.FOR.

Example File 2. Example .3DG file

Test.3DG

```
GRID three-dimensional
TYPE 1
IJK -y +x -z
ORIGIN   .100000000000000E+03   .250000000000000E+03  -.100000000000000E+02
ROTZ  0
DIM  3  6  4
   .000000000000000E+00
   .200000000000000E+01
   .400000000000000E+01
   .700000000000000E+01
   .900000000000000E+01
   .100000000000000E+02
   .000000000000000E+00
   .100000000000000E+01
   .300000000000000E+01
   .600000000000000E+01
   .000000000000000E+00
   .500000000000000E+01
```

```
   .100000000000000E+02
```

The output file is *Test.*3DG which has been overwritten with the following when BLOCK.FOR is run:

Example File 3. Example output (overwritten) .3DG file

Test.3DG

```
GRID THREE-dimensional
TYPE 1
IJK -y +x -z
ORIGIN   .100000000000000E+03   .250000000000000E+03  -.100000000000000E+02
ROTZ  0
DIM  3  6  4
   .000000000000000E+00
   .200000000000000E+01
   .400000000000000E+01
   .700000000000000E+01
   .900000000000000E+01
   .100000000000000E+02
   .000000000000000E+00
   .100000000000000E+01
   .300000000000000E+01
   .600000000000000E+01
   .000000000000000E+00
   .500000000000000E+01
   .100000000000000E+02
MAT
 1 1 1 1 1 1 1 2 2 1 1 3 3 1 1 1 1 3 3 3 3 3 3 2 2 3 3 3 2 2
```

This output .3DG file can then be directly read into GMS to completely define the grid system and the distribution of hydraulic properties. It can be used also to generate a portion of the MODFLOW .BCF file.

2.2 Automatic Generation of Block Centered Flow (BCF) Package

2.2.1. Problem

In modeling three-dimensional groundwater flow and transport in heterogeneous aquifers, the values of hydraulic properties must be accurately assigned to proper grid cells in the numerical model. This task can be time-consuming and prone to error introduction, even with the aid of a powerful pre-processor such as GMS. We have written the program BCF_IN.FOR to efficiently prepare the Block Centered Flow (BCF) package which holds all the information describing the flow system and associated hydraulic properties. The values of some hydraulic properties have to be calculated (e.g., T, S, and leakance) and then input to a selected material block (group of contiguous cells with the same hydraulic properties). This procedure is repeated for all blocks. Completing the .BCF input file manually for a highly heterogeneous aquifer system takes hours, or even a day or more. And again, the laborious process must be repeated to generate a new .BCF file whenever values of the hydraulic properties or block dimensions are changed during subsequent model runs.

2.2.2. Solution

The basic approach of BCF_IN.FOR is to: (1) directly relate the geometric information specifying the material blocks to information on material properties (e.g., MATID, K, Ss and Sy); and (2) automatically calculate and assign values of hydraulic properties (T, S, leakance) to cells of the model. Using the program BCF_IN.FOR, a new .BCF file can be generated in a few seconds when the values of hydraulic properties are changed. The output .BCF file from BCF_IN.FOR can be directly incorporated into the MODFLOW model using the .BCF input file. BCF_IN.FOR is an independent program. However, the most important input information for this program comes from the three-dimensional grid file (*filename*.3DG) generated by GMS.

.

2.2.3. Input Instructions for the BCF_IN.FOR program

Two input files in addition to the .BCF file are required by the BCF_IN.FOR program: a file a .3DG file and a file called MATERIAL.IN

2.2.3.1. Three-Dimensional Grid File (filename.3DG)

In GMS, after three-dimensional grids have been generated and all material blocks defined, the three-dimensional grid file can be obtained by choosing: **File --> Save** and then entering the file name.

2.2.3.2. MATERIAL.IN

In the material property file MATERIAL.IN, list each type of material using one line for each. In each line, first the material type (MATID) is given followed by K, Sy and Ss for that material type.

2.2.4. Example Application

We demonstrate using the BCF_IN.FOR program to generate the .BCF input file for a hypothetical heterogeneous aquifer. This aquifer is composed of five different geological materials: cobble-sand mixture, gravel, clean sand, silty sand, and silt. These materials occur in a patchy (rather than layered) distribution as is common in alluvial aquifers. The simulated volume is about 100 m x 100 m in area and 40 m thick. The solution domain is discretized into 14 columns and 14 rows with variable grid spacing that gradually increases from the center of the domain (where a pumping well is located) to the boundaries. The vertical dimension is divided into three model layers having thicknesses of 8.5 m, 18.5 m, and 13 m respectively, from bottom to top (Figure 2). Material blocks are defined in GMS and the three-dimensional grid file has been saved (select: **File---> Save** and give the filename for .3DG file).

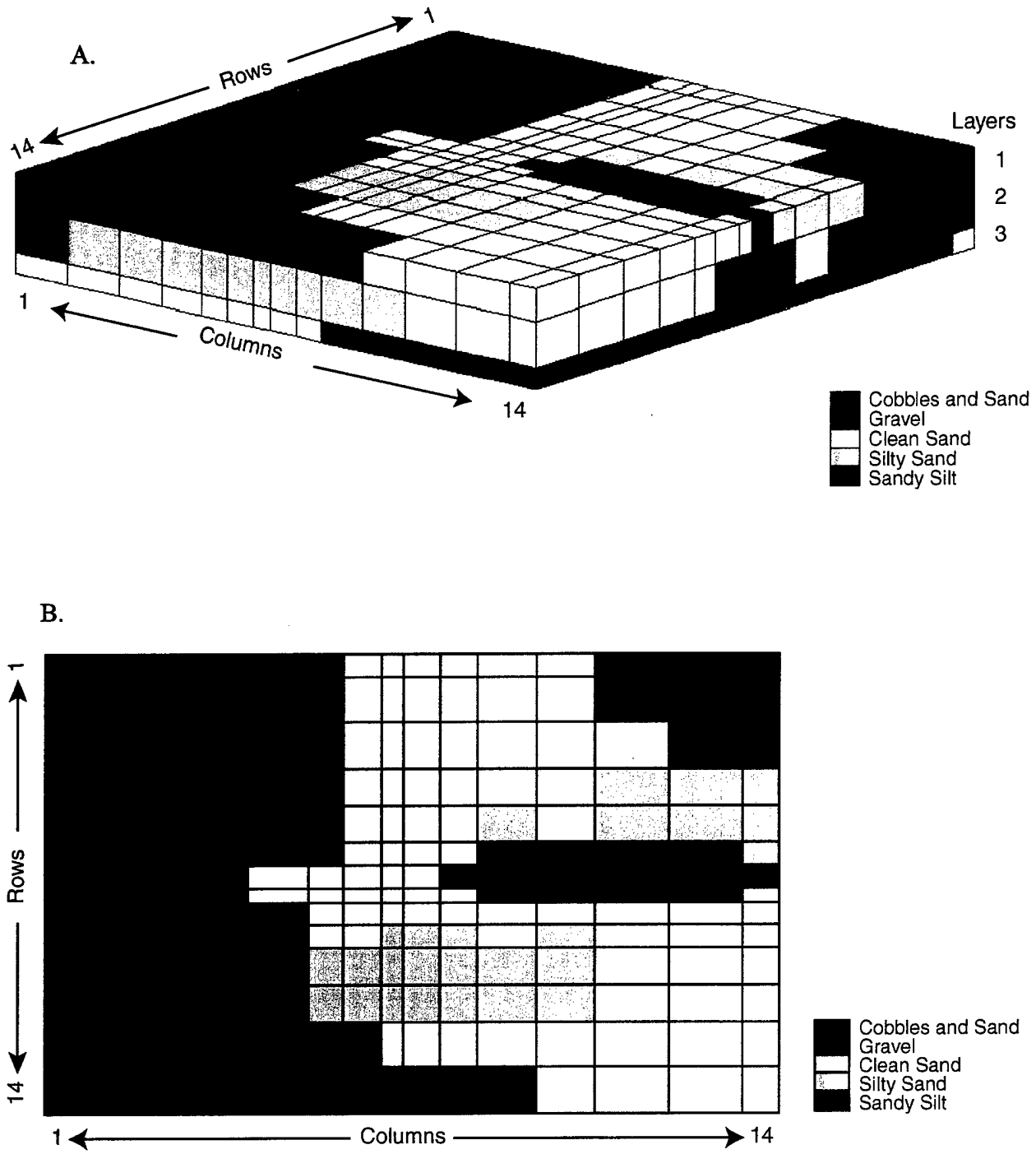
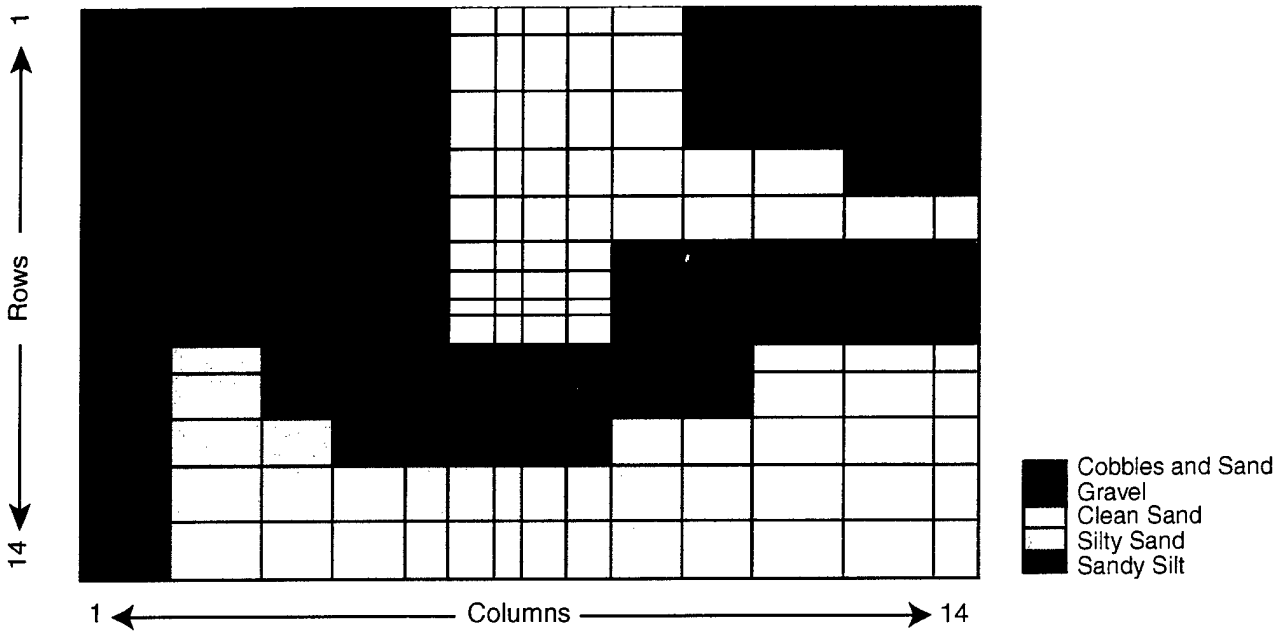


Figure 2. Three-dimensional view and plan views of a heterogeneous aquifer model A. Oblique view of a three-layer three-dimensionally heterogeneous aquifer model with five aquifer material types. B. Plan view of layer 1 (top layer).

C.



D.

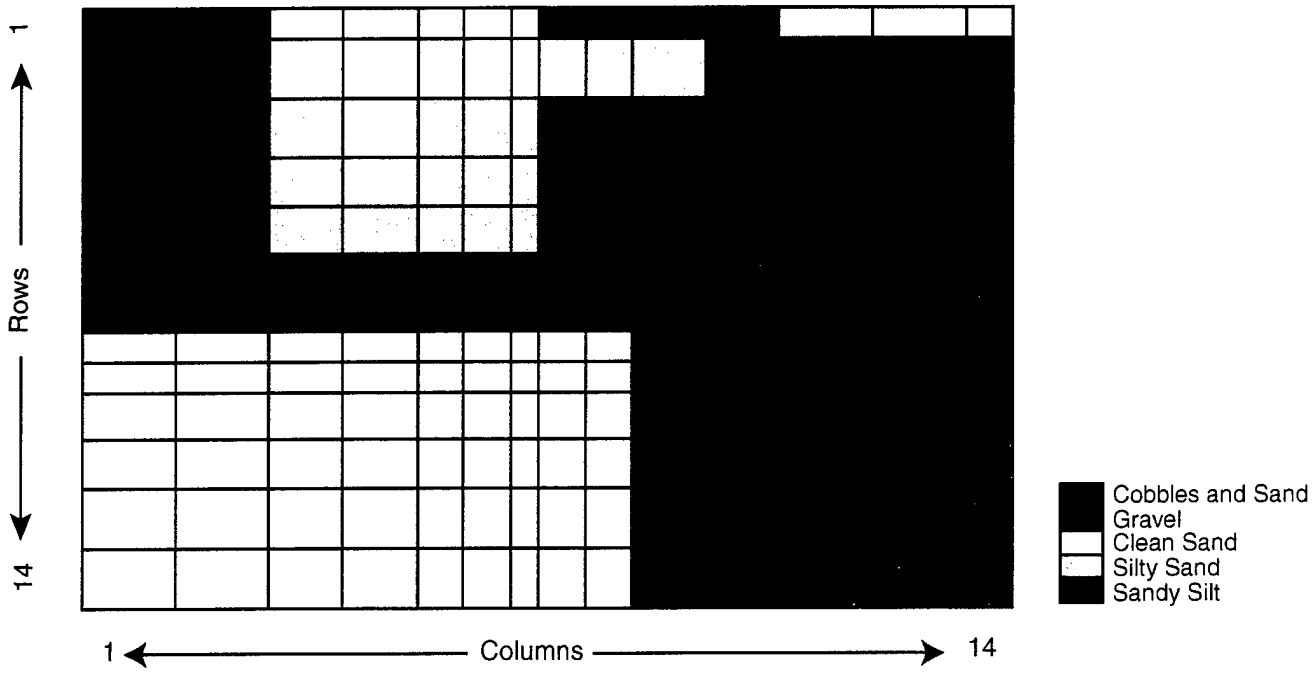


Figure 2. Continued. C. Plan view of layer 2 (middle layer) of the model. D. Plan view of layer 3 (bottom layer) of the model.

Following is the .3DG file saved by GMS for this example application:

Example File 4. Example.3DG file

EXAMPLE.3DG

```
GRID3D
TYPE 1
IJK -y +x -z
ORIGIN 1.000000000000000e+002 2.000000000000000e+002 -4.000000000000000e+001
ROTZ  0
DIM 15 15 4
0.000000000000000e+000
1.000000000000000e+001
2.000000000000000e+001
2.800000000000000e+001
3.600000000000000e+001
4.100000000000000e+001
4.600000000000000e+001
4.900000000000000e+001
5.400000000000000e+001
5.900000000000000e+001
6.700000000000000e+001
7.500000000000000e+001
8.500000000000000e+001
9.500000000000000e+001
1.000000000000000e+002
0.000000000000000e+000
1.000000000000000e+001
2.000000000000000e+001
2.800000000000000e+001
3.600000000000000e+001
4.100000000000000e+001
4.600000000000000e+001
4.900000000000000e+001
5.400000000000000e+001
5.900000000000000e+001
6.700000000000000e+001
7.500000000000000e+001
8.500000000000000e+001
9.500000000000000e+001
1.000000000000000e+002
0.000000000000000e+000
8.500000000000000e+000
2.700000000000000e+001
4.000000000000000e+001
MAT
 3 3 3 3 3 1 1 1 1 1 1 3 3 3 3 3 3 3 3 1 1 1 1 1 1 3 3 3 3 3 3 3 1 1 1 1 1 1 1 3 3 3 3 3 3 1 1 1 1 1 1 2 2 2 3
3 3 3 3 1 1 1 1 2 1 2 2 2 3 3 3 3 3 1 1 1 1 5 5 5 5 2 4 4 4 1 1 1 1 1 5 5 5 5 5 5 4 4 4 1 1 1 1 1 1 5 5 5
 5 1 4 4 4 4 1 1 1 1 1 1 1 1 1 1 4 4 4 4 1 1 2 2 2 1 2 1 1 1 4 4 4 4 2 2 2 2 2 2 2 1 1 1 4 4 4 4 2 2 2 2 2 2 2 1 1
1 4 3 3 3 3 3 1 1 1 1 1 1 1 1 1 4 4 4 3 3 3 3 3 3 3 1 1 1 1 3 3 3 3 3 1 1 1 1 1 5 5 5 5 3 3 3 3 3 1 1 1 1 1
 5 5 5 5 3 3 3 3 3 1 1 1 1 1 5 5 5 5 3 3 3 3 3 3 1 1 1 1 1 1 1 5 5 3 3 3 3 3 3 1 1 1 1 1 1 1 1 1 3 3 3 3 3 1 1 1 1 3 3
3 3 3 4 3 3 3 3 1 1 1 1 3 3 3 3 3 4 3 3 3 3 1 1 1 1 3 3 3 3 3 4 3 3 3 3 1 1 1 1 3 3 3 3 3 4 2 5 5 5 5 5 5
 5 5 5 1 1 1 4 2 5 5 5 5 5 5 5 5 5 1 1 1 4 2 2 2 5 5 5 5 5 5 2 2 1 1 1 4 2 2 2 2 2 2 2 2 2 1 1 1 4 2 2 2 2 2 2 2 2
2 2 1 1 1 5 5 1 1 1 1 1 5 5 5 5 2 2 2 5 5 1 1 1 1 1 2 2 2 4 4 4 4 5 5 2 2 2 2 2 4 4 4 4 4 4 4 5 5 2 2 2 2
 2 4 4 4 4 4 4 4 5 5 2 2 2 2 2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4
4 4 4 4 4 4 4 1 1 1 1 1 1 1 1 1 1 5 5 5 5 5 1 1 1 1 1 1 1 1 1 5 5 5 5 5 1 1 1 1 1 1 1 1 1 5 5 5 5 5 1 1 1 1
 1 1 1 1 1 5 5 5 5 5 1 1 1 1 1 1 1 1 1 1 5 5 5 5 5 1 1 1 1 1 1 1 1 1 1 5 5 5 5 5
```

The first part of this input file consists of geometric information on the location of grid lines for rows, columns, and layers. The second part contains MATIDs (in this case for five materials: 1 through 5), one for each cell in the model grid and each corresponding to the MATID as specified by the example .MAT file described below.

Example File 5. Example .MAT file

EXAMPLE .MAT

```
1       0.02    0.2     5.0e-04
2       0.125   0.21    7.0e-04
3       0.085   0.18    6.0e-05
4       0.01    0.15    9.0e-05
5       0.01    0.23    2.0e-04
```

The original .BCF file that will be taken as input by BCF_IN.FOR also is obtained from GMS when the MODFLOW model domain is generated in GMS and saved there. The data in the original .BCF file will just be read in, and then this file will be overwritten as the new .BCF file with the same name, which now serves as the output file. The following is the initial .BCF file (input to BCF_IN.FOR):

Example File 6. Example .BCF input file

EXAMPLE .BCF

```
        0         0 -888.0000         0 1.0000000         1         0
1 0 0
        0 1.0000000
       11 1.0000000           (10G15.6)        -1
     10.000000      10.000000       8.000000       8.000000       5.000000       5.000000       3.000000       5.000000
    5.000000       8.000000
      8.000000       10.000000      10.000000       5.000000
       11 1.0000000           (10G15.6)        -1
      5.000000       10.000000      10.000000       8.000000       8.000000       5.000000       5.000000       3.000000
    5.000000       5.000000
      8.000000       8.000000       10.000000      10.000000
        0       0.0
        0       0.0
        0       0.0
        0       0.0
        0       0.0
        0       0.0
        0       0.0
        0       0.0
        0       0.0
```

Shown below is the output .BCF file (note it has the same name as the input file) generated by running the BCF_IN.FOR program.

Example File 7. Example .BCF output file

EXAMPLE .BCF

```
        0         0 -888.0000         0 1.0000000         1         0
 1 0 0
        0 1.0000000                             0
       11 1.0000000           (10G15.6)        -1
10.0000         10.0000         8.00000         8.00000         5.00000         5.00000         3.00000         5.00000
5.00000         8.00000
8.00000         10.0000         10.0000         5.00000         .000000
       11 1.0000000           (10G15.6)        -1
5.00000         10.0000         10.0000         8.00000         8.00000         5.00000         5.00000         3.00000
5.00000         5.00000
8.00000         8.00000         10.0000         10.0000         .000000
       11    1.0000           (10G11.4)         0                         Sy of unconfined layer 1
  .1800       .1800       .1800       .1800       .1800       .2000       .2000       .2000       .2000       .2000
  .2000       .1800       .1800       .1800       .1800       .1800       .1800       .1800       .1800       .2000
  .2000       .2000       .2000       .2000       .2000       .1800       .1800       .1800       .1800       .1800
  .1800       .1800       .1800       .2000       .2000       .2000       .2000       .2000       .2000       .2000
  .1800       .1800       .1800       .1800       .1800       .1800       .1800       .2000       .2000       .2000
  .2000       .2000       .2000       .2100       .2100       .2100       .1800       .1800       .1800       .1800
  .1800       .2000       .2000       .2000       .2000       .2100       .2000       .2100       .2100       .2100
  .1800       .1800       .1800       .1800       .1800       .2000       .2000       .2000       .2000       .2300
  .2300       .2300       .2300       .2100       .1500       .1500       .1500       .2000       .2000       .2000
  .2000       .2000       .2300       .2300       .2300       .2300       .2300       .2300       .1500       .1500
  .1500       .2000       .2000       .2000       .2000       .2000       .2000       .2300       .2300       .2300
  .2300       .2000       .1500       .1500       .1500       .1500       .2000       .2000       .2000       .2000
  .2000       .2000       .2000       .2000       .2000       .2000       .1500       .1500       .1500       .1500
  .2000       .2000       .2100       .2100       .2100       .2000       .2100       .2000       .2000       .2000
  .1500       .1500       .1500       .1500       .2100       .2100       .2100       .2100       .2100       .2100
  .2100       .2000       .2000       .2000       .1500       .1500       .1500       .1500       .2100       .2100
  .2100       .2100       .2100       .2100       .2100       .2000       .2000       .2000       .1500       .1800
  .1800       .1800       .1800       .1800       .2000       .2000       .2000       .2000       .2000       .2000
  .2000       .2000       .1500       .1500       .1500       .1800       .1800       .1800       .1800       .1800
  .1800       .1800       .2000       .2000       .2000       .2000
       11    1.0000           (10G11.4)         0                         K of unconfined layer 1
.8500E-01   .8500E-01   .8500E-01   .8500E-01   .8500E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01
.2000E-01   .8500E-01   .8500E-01   .8500E-01   .8500E-01   .8500E-01   .8500E-01   .8500E-01   .8500E-01   .2000E-01
.2000E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01   .8500E-01   .8500E-01   .8500E-01   .8500E-01   .8500E-01
.8500E-01   .8500E-01   .8500E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01
.8500E-01   .8500E-01   .8500E-01   .8500E-01   .8500E-01   .8500E-01   .8500E-01   .2000E-01   .2000E-01   .2000E-01
.2000E-01   .2000E-01   .2000E-01   .1250       .1250       .1250       .8500E-01   .8500E-01   .8500E-01   .8500E-01
.8500E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01   .1250       .2000E-01   .1250       .1250       .1250
.8500E-01   .8500E-01   .8500E-01   .8500E-01   .8500E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01   .1000E-01
.1000E-01   .1000E-01   .1000E-01   .1250       .1000E-01   .1000E-01   .1000E-01   .2000E-01   .2000E-01   .2000E-01
.2000E-01   .2000E-01   .1000E-01   .1000E-01   .1000E-01   .1000E-01   .1000E-01   .1000E-01   .1000E-01   .1000E-01
.1000E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01   .1000E-01   .1000E-01   .1000E-01
.1000E-01   .2000E-01   .1000E-01   .1000E-01   .1000E-01   .1000E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01
.2000E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01   .1000E-01   .1000E-01   .1000E-01   .1000E-01
.2000E-01   .2000E-01   .1250       .1250       .1250       .2000E-01   .1250       .2000E-01   .2000E-01   .2000E-01
.1000E-01   .1000E-01   .1000E-01   .1000E-01   .1250       .1250       .1250       .1250       .1250       .1250
.1250       .2000E-01   .2000E-01   .2000E-01   .1000E-01   .1000E-01   .1000E-01   .1000E-01   .1250       .1250
.1250       .1250       .1250       .1250       .1250       .2000E-01   .2000E-01   .2000E-01   .1000E-01   .8500E-01
.8500E-01   .8500E-01   .8500E-01   .8500E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01
.2000E-01   .2000E-01   .1000E-01   .1000E-01   .1000E-01   .8500E-01   .8500E-01   .8500E-01   .8500E-01   .8500E-01
.8500E-01   .8500E-01   .2000E-01   .2000E-01   .2000E-01   .2000E-01
        0  -13.0000                                                    Bottom elevation of unconfined layer 1
       11    1.0000           (10G11.4)         0                         Leakance of unconfined layer 1
.5397E-02   .5397E-02   .5397E-02   .5397E-02   .5397E-02   .1270E-02   .1270E-02   .1270E-02   .1270E-02   .1270E-02
.8000E-03   .9985E-03   .9985E-03   .9985E-03   .5397E-02   .5397E-02   .5397E-02   .5397E-02   .5397E-02   .1270E-02
```

```
.1270E-02  .1270E-02  .1270E-02  .1270E-02  .8000E-03  .9985E-03  .9985E-03  .9985E-03  .5397E-02  .5397E-02
.5397E-02  .5397E-02  .5397E-02  .1270E-02  .1270E-02  .1270E-02  .1270E-02  .1270E-02  .8000E-03  .8000E-03
.9985E-03  .9985E-03  .5397E-02  .5397E-02  .5397E-02  .5397E-02  .5397E-02  .1270E-02  .1270E-02  .1270E-02
.1270E-02  .1270E-02  .1270E-02  .1944E-02  .1024E-02  .1024E-02  .5397E-02  .5397E-02  .5397E-02  .5397E-02
.5397E-02  .1270E-02  .1270E-02  .1270E-02  .1270E-02  .1270E-02  .1944E-02  .1270E-02  .1944E-02  .1944E-02
.5397E-02  .5397E-02  .5397E-02  .5397E-02  .5397E-02  .1270E-02  .1270E-02  .1270E-02  .1270E-02  .1318E-02
.1318E-02  .1318E-02  .1318E-02  .6218E-02  .6349E-03  .1318E-02  .1318E-02  .2305E-02  .2305E-02  .1270E-02
.1270E-02  .1270E-02  .8989E-03  .1318E-02  .1318E-02  .1318E-02  .1318E-02  .1318E-02  .6349E-03  .1318E-02
.1318E-02  .2305E-02  .2305E-02  .1270E-02  .1270E-02  .1270E-02  .1270E-02  .1318E-02  .1318E-02  .1318E-02
.1318E-02  .2305E-02  .6349E-03  .1318E-02  .1318E-02  .1318E-02  .2305E-02  .1270E-02  .1270E-02  .1270E-02
.1270E-02  .2305E-02  .2305E-02  .2305E-02  .2305E-02  .2305E-02  .6349E-03  .1381E-02  .6349E-03  .6349E-03
.8000E-03  .8000E-03  .1024E-02  .1024E-02  .1024E-02  .8000E-03  .1024E-02  .1270E-02  .1270E-02  .1270E-02
.6349E-03  .1381E-02  .6349E-03  .6349E-03  .1024E-02  .1024E-02  .1024E-02  .1024E-02  .1024E-02  .1024E-02
.1024E-02  .1270E-02  .1270E-02  .1270E-02  .6349E-03  .1381E-02  .1381E-02  .6349E-03  .1024E-02  .1024E-02
.1024E-02  .1024E-02  .1024E-02  .7937E-02  .7937E-02  .1270E-02  .1270E-02  .1270E-02  .6349E-03  .6646E-02
.6646E-02  .6646E-02  .6646E-02  .6646E-02  .2506E-02  .2506E-02  .2506E-02  .2506E-02  .2506E-02  .1270E-02
.1270E-02  .1270E-02  .6349E-03  .1381E-02  .1381E-02  .6646E-02  .6646E-02  .6646E-02  .6646E-02  .6646E-02
.6646E-02  .6646E-02  .2506E-02  .1270E-02  .1270E-02  .1270E-02
      11    1.0000          (10G11.4)          0                          Ss of confined layer 2
.6000E-04  .6000E-04  .6000E-04  .6000E-04  .6000E-04  .5000E-03  .5000E-03  .5000E-03  .5000E-03  .5000E-03
.2000E-03  .2000E-03  .2000E-03  .2000E-03  .6000E-04  .6000E-04  .6000E-04  .6000E-04  .6000E-04  .5000E-03
.5000E-03  .5000E-03  .5000E-03  .5000E-03  .2000E-03  .2000E-03  .2000E-03  .2000E-03  .6000E-04  .6000E-04
.6000E-04  .6000E-04  .6000E-04  .5000E-03  .5000E-03  .5000E-03  .5000E-03  .5000E-03  .2000E-03  .2000E-03
.2000E-03  .2000E-03  .6000E-04  .6000E-04  .6000E-04  .6000E-04  .6000E-04  .5000E-03  .5000E-03  .5000E-03
.5000E-03  .5000E-03  .5000E-03  .5000E-03  .2000E-03  .2000E-03  .6000E-04  .6000E-04  .6000E-04  .6000E-04
.6000E-04  .5000E-03  .5000E-03  .5000E-03  .5000E-03  .5000E-03  .5000E-03  .5000E-03  .5000E-03  .5000E-03
.6000E-04  .6000E-04  .6000E-04  .6000E-04  .6000E-04  .5000E-03  .5000E-03  .5000E-03  .5000E-03  .6000E-04
.6000E-04  .6000E-04  .6000E-04  .6000E-04  .9000E-04  .6000E-04  .6000E-04  .6000E-04  .6000E-04  .5000E-03
.5000E-03  .5000E-03  .5000E-03  .6000E-04  .6000E-04  .6000E-04  .6000E-04  .6000E-04  .9000E-04  .6000E-04
.6000E-04  .6000E-04  .6000E-04  .5000E-03  .5000E-03  .5000E-03  .5000E-03  .6000E-04  .6000E-04  .6000E-04
.6000E-04  .6000E-04  .9000E-04  .6000E-04  .6000E-04  .6000E-04  .6000E-04  .5000E-03  .5000E-03  .5000E-03
.5000E-03  .6000E-04  .6000E-04  .6000E-04  .6000E-04  .6000E-04  .9000E-04  .7000E-03  .2000E-03  .2000E-03
.2000E-03  .2000E-03  .2000E-03  .2000E-03  .2000E-03  .2000E-03  .2000E-03  .5000E-03  .5000E-03  .5000E-03
.9000E-04  .7000E-03  .2000E-03  .2000E-03  .2000E-03  .2000E-03  .2000E-03  .2000E-03  .2000E-03  .2000E-03
.2000E-03  .5000E-03  .5000E-03  .5000E-03  .9000E-04  .7000E-03  .7000E-03  .2000E-03  .2000E-03  .2000E-03
.2000E-03  .2000E-03  .2000E-03  .7000E-03  .7000E-03  .5000E-03  .5000E-03  .5000E-03  .9000E-04  .7000E-03
.7000E-03  .7000E-03  .7000E-03  .7000E-03  .7000E-03  .7000E-03  .7000E-03  .7000E-03  .7000E-03  .5000E-03
.5000E-03  .5000E-03  .9000E-04  .7000E-03  .7000E-03  .7000E-03  .7000E-03  .7000E-03  .7000E-03  .7000E-03
.7000E-03  .7000E-03  .7000E-03  .5000E-03  .5000E-03  .5000E-03
      11    1.0000          (10G11.4)          0                          T of confined layer 2
1.572      1.572      1.572      1.572      1.572      .3700      .3700      .3700      .3700      .3700
.1850      .1850      .1850      .1850      1.572      1.572      1.572      1.572      1.572      .3700
.3700      .3700      .3700      .3700      .1850      .1850      .1850      .1850      1.572      1.572
1.572      1.572      1.572      .3700      .3700      .3700      .3700      .3700      .1850      .1850
.1850      .1850      1.572      1.572      1.572      1.572      1.572      .3700      .3700      .3700
.3700      .3700      .3700      .3700      .1850      .1850      1.572      1.572      1.572      1.572
1.572      .3700      .3700      .3700      .3700      .3700      .3700      .3700      .3700      .3700
1.572      1.572      1.572      1.572      1.572      .3700      .3700      .3700      .3700      1.572
1.572      1.572      1.572      1.572      .1850      1.572      1.572      1.572      1.572      .3700
.3700      .3700      .3700      1.572      1.572      1.572      1.572      1.572      .1850      1.572
1.572      1.572      1.572      .3700      .3700      .3700      .3700      1.572      1.572      1.572
1.572      1.572      .1850      1.572      1.572      1.572      1.572      .3700      .3700      .3700
.3700      1.572      1.572      1.572      1.572      1.572      .1850      2.313      .1850      .1850
.1850      .1850      .1850      .1850      .1850      .1850      .1850      .3700      .3700      .3700
.1850      2.313      .1850      .1850      .1850      .1850      .1850      .1850      .1850      .1850
.1850      .3700      .3700      .3700      .1850      2.313      2.313      .1850      .1850      .1850
.1850      .1850      .1850      2.313      2.313      .3700      .3700      .3700      .1850      2.313
2.313      2.313      2.313      2.313      2.313      2.313      2.313      2.313      2.313      .3700
.3700      .3700      .1850      2.313      2.313      2.313      2.313      2.313      2.313      2.313
2.313      2.313      2.313      .3700      .3700      .3700
      11    1.0000          (10G11.4)          0                          Leakance of confined layer 2
.1873E-02  .1873E-02  .3112E-02  .3112E-02  .3112E-02  .1481E-02  .1481E-02  .1127E-02  .1127E-02  .1127E-02
.7407E-03  .1043E-02  .1043E-02  .1043E-02  .1873E-02  .1873E-02  .3112E-02  .3112E-02  .3112E-02  .1481E-02
```

.1481E-02 .2014E-02 .2014E-02 .2014E-02 .7407E-03 .7407E-03 .7407E-03 .7407E-03 .1873E-02 .1873E-02
.7002E-02 .7002E-02 .7002E-02 .2014E-02 .2014E-02 .1127E-02 .1127E-02 .1127E-02 .7407E-03 .7407E-03
.7407E-03 .7407E-03 .1873E-02 .1873E-02 .7002E-02 .7002E-02 .7002E-02 .2014E-02 .2014E-02 .1127E-02
.1127E-02 .1127E-02 .1127E-02 .1127E-02 .7407E-03 .7407E-03 .1873E-02 .1873E-02 .7002E-02 .7002E-02
.7002E-02 .2014E-02 .2014E-02 .1127E-02 .1127E-02 .1127E-02 .1127E-02 .1127E-02 .1127E-02 .1127E-02
.1873E-02 .1873E-02 .1873E-02 .1873E-02 .1873E-02 .1127E-02 .1127E-02 .1127E-02 .1127E-02 .1873E-02
.1873E-02 .1873E-02 .1873E-02 .1873E-02 .7407E-03 .1873E-02 .1873E-02 .1873E-02 .1873E-02 .1127E-02
.1127E-02 .1127E-02 .1127E-02 .1873E-02 .1873E-02 .1873E-02 .1873E-02 .1873E-02 .7407E-03 .1873E-02
.1873E-02 .1873E-02 .1873E-02 .1127E-02 .1127E-02 .1127E-02 .1127E-02 .1873E-02 .1873E-02 .1873E-02
.1873E-02 .1873E-02 .8791E-03 .3112E-02 .3112E-02 .3112E-02 .3112E-02 .1481E-02 .1481E-02 .1481E-02
.1481E-02 .1873E-02 .1873E-02 .1873E-02 .1873E-02 .1873E-02 .8791E-03 .3490E-02 .8791E-03 .8791E-03
.8791E-03 .8791E-03 .8791E-03 .8791E-03 .8791E-03 .7407E-03 .7407E-03 .1127E-02 .1127E-02 .1127E-02
.8791E-03 .3490E-02 .8791E-03 .8791E-03 .8791E-03 .8791E-03 .8791E-03 .8791E-03 .8791E-03 .7407E-03
.7407E-03 .1127E-02 .1127E-02 .1127E-02 .8791E-03 .3490E-02 .3490E-02 .8791E-03 .8791E-03 .8791E-03
.8791E-03 .8791E-03 .8791E-03 .2004E-02 .2004E-02 .1127E-02 .1127E-02 .1127E-02 .8791E-03 .3490E-02
.3490E-02 .3490E-02 .3490E-02 .3490E-02 .3490E-02 .3490E-02 .3490E-02 .2004E-02 .2004E-02 .1127E-02
.1127E-02 .1127E-02 .8791E-03 .3490E-02 .3490E-02 .3490E-02 .3490E-02 .3490E-02 .3490E-02 .3490E-02
.3490E-02 .2004E-02 .2004E-02 .1127E-02 .1127E-02 .1127E-02

11 1.0000 (10G11.4) 0 **Ss of confined layer 3**

.2000E-03 .2000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .2000E-03 .2000E-03 .2000E-03
.2000E-03 .7000E-03 .7000E-03 .7000E-03 .2000E-03 .2000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03
.5000E-03 .7000E-03 .7000E-03 .7000E-03 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .2000E-03 .2000E-03
.7000E-03 .7000E-03 .7000E-03 .7000E-03 .7000E-03 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04
.9000E-04 .9000E-04 .2000E-03 .2000E-03 .7000E-03 .7000E-03 .7000E-03 .7000E-03 .7000E-03 .9000E-04
.9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .2000E-03 .2000E-03 .7000E-03 .7000E-03
.7000E-03 .7000E-03 .7000E-03 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04
.9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04
.9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04
.9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04
.9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04 .9000E-04
.9000E-04 .9000E-04 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03
.5000E-03 .2000E-03 .2000E-03 .2000E-03 .2000E-03 .2000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03
.5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .2000E-03 .2000E-03 .2000E-03 .2000E-03 .2000E-03
.5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .2000E-03
.2000E-03 .2000E-03 .2000E-03 .2000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03
.5000E-03 .5000E-03 .5000E-03 .2000E-03 .2000E-03 .2000E-03 .2000E-03 .2000E-03 .5000E-03 .5000E-03
.5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .2000E-03 .2000E-03 .2000E-03
.2000E-03 .2000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03 .5000E-03
.5000E-03 .2000E-03 .2000E-03 .2000E-03 .2000E-03 .2000E-03

11 1.0000 (10G11.4) 0 **T of confined layer 3**

.8500E-01 .8500E-01 .1700 .1700 .1700 .1700 .1700 .8500E-01 .8500E-01 .8500E-01
.8500E-01 1.063 1.063 1.063 .8500E-01 .8500E-01 .1700 .1700 .1700 .1700
.1700 1.063 1.063 1.063 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01
1.063 1.063 1.063 1.063 1.063 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01
.8500E-01 .8500E-01 .8500E-01 .8500E-01 1.063 1.063 1.063 1.063 1.063 .8500E-01
.8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 1.063 1.063
1.063 1.063 1.063 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01
.8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01
.8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01
.8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01
.8500E-01 .8500E-01 .1700 .1700 .1700 .1700 .1700 .1700 .1700 .1700
.1700 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .1700 .1700 .1700 .1700
.1700 .1700 .1700 .1700 .1700 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01
.1700 .1700 .1700 .1700 .1700 .1700 .1700 .1700 .1700 .8500E-01
.8500E-01 .8500E-01 .8500E-01 .8500E-01 .1700 .1700 .1700 .1700 .1700 .1700
.1700 .1700 .1700 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .1700 .1700
.1700 .1700 .1700 .1700 .1700 .1700 .1700 .8500E-01 .8500E-01 .8500E-01
.8500E-01 .8500E-01 .1700 .1700 .1700 .1700 .1700 .1700 .1700 .1700
.1700 .8500E-01 .8500E-01 .8500E-01 .8500E-01 .8500E-01

2.3. Automatic Generation of the Well Package for Wells Open to Multiple Layers

2.3.1. Problem

A pumping well may be screened across several geologic or hydrostratigraphic layers having different hydraulic properties, or several model layers in a numerical model such as MODFLOW that have the same or different hydraulic properties. The pumping rate of a well is comprised of the sum of the flow rates of all the geologic or model layers contributing to the well discharge. In MODFLOW the pumping rate (the strength of the sink term) must be specified for each individual model layer. It is apparent that the pumping rate for a well in an individual layer is a fraction of the total pumping rate of the well. In practice, fractional pumping rates for individual layers have been approximated (e.g., Javandel and Witherspoon, 1969; Molz et al., 1990; McDonald and Harbaugh, 1998 eq. 68) by apportioning flow based on the relative transmissivity of the contributing layers (Figure 3). Currently, the MODFLOW user must calculate the individual pumping rates per well cell, representing the fractional contribution for a given layer, for each time period that has a different pumping rate. The calculations must be repeated if model parameter values or grid configuration are changed. Performing such calculations by hand can be time-consuming and error-prone.

2.3.2. Solution

A simple algorithm is implemented in the program WELL_Q.FOR to apportion flow rates by layer based on: (1) values of T designated for active pumping cells; and (2) total Q for a given period. The assumption behind this approach is that the drawdown in the pumping well is uniform throughout the well so that an aquifer or model layer having a relatively large transmissivity value contributes a higher flow rate to the total pumping rate than layers with lower T. Based on this assumption, the fraction of the total pumping rate contributed by a well in an individual model layer can be calculated by the following equation:

$$Q_i = \frac{T_i}{\sum_{j=1}^{n} T_j} Q$$

where n is the number of model layers contributing to the well (for example, $n = 5$ for the well shown in Figure 3), i is the layer for which Q_i of the well is being calculated and the summation, T_j, gives the combined transmissivity of all layers open to the well.

2.3.3. Input Instructions for the WELL_Q.FOR Program

Two input files must be provided for the WELL_Q.FOR program: WELL.IN and Q_TIME.

2.3.3.1. WELL.IN

This file (see Example File 8) provides the model layer number having an active well cell, the hydraulic conductivity (K) of the layer, and the thickness of this layer. For each multilayer well, the WELL.IN file has one line for each layer in the model that has an active well cell.

2.3.3.2. Q_TIME

In this file (see Example File 9), NCOL (column number) and NROW (row number) of the pumping well are given on the first line. Then, one line is given for each stress period with the first number on the line being the stress period sequence number, and the second number on the line being the pumping rate for that stress period in consistent units. The pumping rate value in Q_TIME follows the MODFLOW sign convention with negative value for pumping (sink), or positive values for injection (source).

2.3.4. Example Application

This example demonstrates the use of the WELL_Q.FOR program for generating the well package for a MODFLOW model with a well pumping in a shallow heterogeneous aquifer. A model domain of 250 ft x 250 ft x 58 ft was discretized into 65 rows, 65 columns, and 28 layers. The pumping well consists of cells in three model layers (layers 21 to 23) in NCOL = 33 and NROW = 33. As in many real circumstances, the pumping rate in this model scenario fluctuates at early time. To account for this early-time variable pumping rate, six stress periods are used. Input files for this example are given below:

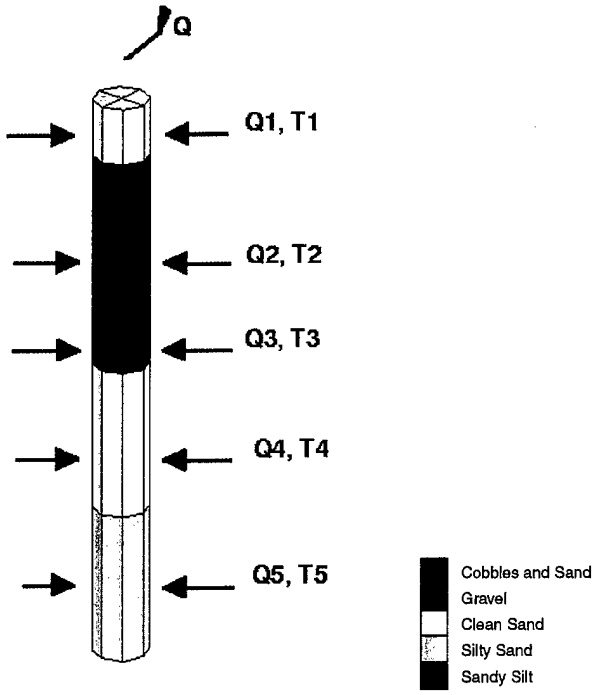


Figure 3. Schematic diagram of a pumping well screened on five layers

Example File 8. Example WELL.IN file

WELL.IN

```
21      0.125  1.25
```

```
22        0.225  2.0
23        0.225  1.0
```

Example File 9. Example Q_TIME file

Q_TIME

```
33   33
1 -0.35
2 -1.200000
3 -1.800000
4 -2.47000000
5 -0.200000
6 -2.4700000
```

The output file of the WELL_Q.FOR program is the well package file for MODFLOW:

Example File 10. Example VARIABLE.WEL file

VARIABLE.WEL

```
 3          0
 3
21         33         33  -.065789
22         33         33  -.189474
23         33         33  -.094737
 3
21         33         33  -.225564
22         33         33  -.649624
23         33         33  -.324812
 3
21         33         33  -.338346
22         33         33  -.974436
23         33         33  -.487218
 3
21         33         33  -.464286
22         33         33 -1.337143
23         33         33  -.668571
 3
21         33         33  -.037594
22         33         33  -.108271
23         33         33  -.054135
 3
21         33         33  -.464286
22         33         33 -1.337143
23         33         33  -.668571
```

2.4. Output of Drawdown for Observation Wells

2.4.1. Problem

MODFLOW output provides drawdown values for every active node in the model domain at each time step of a model run. Although GMS has been designed to be able to retrieve drawdown values for an observation point from MODFLOW model runs through the GAGE function, it is required that model-calculated drawdown be saved for every time step. As a result, the saved drawdown output file, even in binary form, can be quite large; ASCII Text files on the order of 50 to 100 MB are not unusual for a three-dimensional model having a hundred thousand cells or more. For

some modeling activities such as matching drawdown behavior at pumping and/or observation wells, simulated drawdown results are needed at these particular wells rather than throughout the full flow domain - so the complete set of drawdown results for a given run would not be needed.

2.4.2. Solution

To reduce the amount of writing to disk and the size of the drawdown file, we developed the OBSERV.FOR routine for recording the drawdown versus time data only at specified observation points or cells, rather than at all cells. This is implemented within MODFLOW, and is activated through minor modifications to the GMS super file and the MODFLOW .BAS file (described in detail below in section 2.4.6.). The user specifies the needed observation points using either row, column, and layer specifications or absolute coordinates. The OBSERV.FOR routine uses the coordinate transformation specification contained in the MODFLOW .MFS file to convert from coordinate positions to row, column, layer indices.

2.4.3 Input Instructions for OBSERV.FOR

2.4.3.1 The .OBI File

The inputs for the OBSERV.FOR routine are the locations of well cells of interest placed in a file commonly using the suffix .OBI. The locations of well cells can be represented by either the cell row, column, layer indices or the x, y, z coordinates of an observation point, or well cells. Wells that intercept multiple model layers have cell location data for each layer. The format for the .OBI file is:

```
    NOBS,        OPTION
For each NOBS well layer if OPTION = 0
    I J K
For each NOBS well if OPTION < 0
    X Y Z
For each NOBS well if OPTION > 0
    X Y K
```

Where

NOBS - Number of observation locations

OPTION - 0 -> Integer row, column and layer specification
<0 -> x , y, z coordinate positions
>0 -> x, y coordinate locations with K as an integer layer specification

I, J, K INTEGER row, column and layer specification respectively

X, Y, Z REAL coordinates

2.4.4. Application Example

The use of the OBSERV.FOR routine is illustrated using test case 1 of the MODFLOWP user's manual (Hill, 1992). The pumping well is located at row 9 column 10. The domain contains two layers with 18 rows and columns. The horizontal cell widths are 1,000 ft on each side. The layers are 50 ft thick separated by a 10 ft thick aquitard that is not explicitly represented in the model. The

well penetrates both model layers. The default GMS axis definitions of x corresponding to J (columns) and y corresponding to I (rows) are used. X increases with increasing J and y decreases with increasing I. These relationships of the coordinate axes to the row and column indices are defined in the GMS .MFS MODFLOW superfile (See Example file 15). Below is the .OBI input file for OBSERV.FOR using cell numbers for this example:

Example File 11. Example .OBI file using cell numbers

```
2, 0
9, 10, 1
9, 10, 1
```

And below is the corresponding .OBI file for the same well cells if the coordinates of the well cells are used instead of the cell numbers:

Example File 12. Example .OBI file using coordinates

```
2,-1
9500., 9500. , -40.
9500., 9500. , -75.
```

All inputs in the .OBI file are free format. If coordinates are used, they need only lie within the cell; they do not have to exactly match the coordinates of the cell node. The well coordinates option may be most useful when the model grid geometry is irregular and/or when the geometry is changed for subsequent model runs - because then one does not need to update the row, column, and layer numbers for the observation points.

The output using Example file 12 is listed below as Example file 13. The input information and GMS coordinate transformation are listed at the top. The first column well cell data is the time step (KSTP), second the stress period (KPER), third the elapsed time since the start of pumping (T_TOTAL). The next columns are calculated drawdown for each well cell. The cell numbers are listed on the top of each column.

2.4.5. Weighted Drawdown Based on Transmissivity

Because the model equivalent of field-observed drawdown is a combined drawdown of the cells of all the layers open to the well, a weighted drawdown has to be calculated for comparison of model and observed results. This is done by calculating a weighted drawdown for the pumping or observation well based on the values of transmissivity (T_j) of the involved cells (e.g., Javandel and Witherspoon, 1969). For example, if a well is screened in n cells, the drawdown in that well (s) may be calculated as the sum of the weighted drawdown in the contributing n cells:

$$s = \sum_{j=1}^{n} \frac{s_j T_j}{T}$$

where T is the sum of the transmissivity (T_j) values of all screened cells. Note that the cells are not

necessarily vertically adjacent to each other - the layers open to a well can be separated by blank or cased intervals. However, they should have the same horizontal coordinates (i.e., their column and row numbers, respectively, should be the same).

Example File 13. Example of .OBO file

```
 Observation location drawdown
   2    cells using option  -1
 9500.       9500.      -40.00
 9500.       9500.      -70.00
IJK -y +x -z
 ORIG    0.000000E+00    0.000000E+00     -100.000000
 ROTZ    0.000000E+00
 Observation cell drawdown
 KSTP   KPER   T_TOTAL ROW=  9  ROW=  9
                       COL= 10  COL= 10
                       LAY=  1  LAY=  2
   1      1   1.000     .9853E-03 .9992E-02
   1      2   4.000     .3942E-02 .3991E-01
   1      3   10.00     .9859E-02 .9953E-01
   1      4   23.12     .2281E-01 .2288
   2      4   38.86     .3838E-01 .3824
   3      4   57.74     .5709E-01 .5645
   4      4   80.41     .7959E-01 .7800
   5      4   107.6     .1067     1.034
   6      4   140.2     .1392     1.333
   7      4   179.4     .1784     1.684
   8      4   226.4     .2256     2.093
   9      4   282.8     .2825     2.567
 Weighted average drawdown of multilayer wells
 KSTP   KPER   T_TOTAL ROW=  9
                       COL= 10
   1      1   1.000     .4181E-02
   1      2   4.000     .1671E-01
   1      3   10.00     .4168E-01
   1      4   23.12     .9590E-01
   2      4   38.86     .1604
   3      4   57.74     .2371
   4      4   80.41     .3281
   5      4   107.6     .4358
   6      4   140.2     .5630
   7      4   179.4     .7126
   8      4   226.4     .8881
   9      4   282.8     1.093
```

2.4.6. Notes on Usage with GMS

The OBSERV.FOR routine is included in the modified version of MODFLOW that accompanies this report. To activate this modified MODFLOW code, the following additional files and modifications must be made:

1. Establish the input file named: *prefix*.OBI (see section 2.4.4 above)
2. Edit the MODFLOW super file, *prefix*.MFS, generated by GMS in the following ways:
   a) Add the following two lines in the file list:
      OBIN 31 *prefix*.OBI
      OBOT 32 *prefix*.OBO
      NOTE: In these two new lines, 31 and 32 are FORTRAN unit numbers; any numbers can be used as long as they do not conflict with other assigned unit

numbers. Besides those listed in the .BAS file and .MFS files, FORTRAN unit numbers 98 and 99 are reserved for a temporary scratch file and the .MFS file respectively.

b) Put single quotation marks around the word: ORIG (see Example File 14 below).

3. Edit line 4 of the .BAS file by activating IUNIT number 17 for the input file (31) and IUNIT number 21 for the output file (32) to be used by .OBI and .OBO files, respectively (see Example File 15 below).

The following example is the part of the GMS super file for MODFLOW which illustrates the changes described above:

Example File 14. Example modified .MFS file

```
MODSUP
IJK -y +x -z
LIST   26 "two_layer_trans.out"
BAS1    1 "two_layer_trans.bas"
BCF3   11 "two_layer_trans.bcf"
OUT1   10 "two_layer_trans.oc"
HEAD  -30 "two_layer_trans.hed"
DRAW  -35 "two_layer_trans.drw"
CCF   -40 "two_layer_trans40.ccf"
PCG2   12 "two_layer_trans.pcg"
RIV1   15 "two_layer_trans.riv"
WEL1   13 "two_layer_trans.wel"
GHB1   16 "two_layer_trans.ghb"
RCH1   20 "two_layer_trans.rch"
MT three-dimensional  -29 "two_layer_trans.hff"
OBIN   31 "two_layer_trans.obi"
OBOT   32 "two_layer_trans.obo"
'ORIG' 0.000000000000000e+000 0.000000000000000e+000 -1.00000000000000e+002
ROTZ 0
LAYER   0       50.000000 (10G15.6)
DMAT 1
MPSC 1 0 0
MTRN 1 0 0
MHC 1 0 0
MBE 1 0 0
MLK 1 0 0
MSSC 1 0 0
MTE 1 0 0
MWDF 1 0 0
```

Example File 15. Top of modified .BAS file

```
MODULAR MODEL - TWO_LAYER EXAMPLE PROBLEM

        2       18       18        4        4
 11 13  0 15  0  0 16 20  0  0  0 10 12  0  0  0 31  0  0  0 32 29  0  0
        0        1
        0        1
        0        1
 -999.0000
        1 1.0000000          (10G15.6)         0
                      :
```

@@@ Modified line

2.4.7. Notes on Usage with MODFLOWP

At the time this report was written, GMS used the 9/1/87 version of MODFLOW 88 and the latest version of MODFLOWP (3.2) used the 5/23/96 version of MODFLOW 96. One of the differences between MODFLOW 88 and MODFLOW 96 is the method used to open files. To activate the OBSERV.FOR routine in the modified MODFLOWP program do the following:

1. Establish the input file named: *prefix*.OBI (see section 2.4.4 above)
2. Add the following two lines in the NAME FILE:

   OBIN 31 path*prefix*.OBI
   OBOT 32 path*prefix*.OBO
   NOTE: In these two new lines, 31 and 32 are FORTRAN unit numbers; any numbers can be used as long as they do not conflict with other assigned unit numbers. Besides the FORTRAN unit numbers listed in the NAME FILE, unit numbers 0 and 96 through 99 are reserved in MODFLOWP.

3. MODIFICATIONS TO MODFLOWP

The above sections present our modifications to MODFLOW which runs the forward simulation for the groundwater flow problem. That is, when a hydrogeologic system is discretized into a model structure with hydraulic parameters and boundary conditions, MODFLOW solves for head or drawdown and flux distributions in time and space. If the model structure is reasonable, values of parameters are accurate, and the initial and boundary conditions are defined correctly, one may expect that the calculated solutions (head and flux) will match or closely approximate the observed head and flux. However, it is exceedingly rare to have enough data to determine "true" values of aquifer parameters for a hydrogeologic system, and boundary conditions are even more difficult to determine. As a result, calculated results usually deviate from the observed data. Satisfactory modeling results may often be obtained only after many trial-and-error changes to system parameters and boundary conditions. The changes usually rely on the modeler's knowledge of hydrogeology, degree of familiarity with the simulated area, and professional judgment. The decision about when a satisfactory, or the best, model has been achieved largely depends on the modeler's subjectivity. The trial-and-error process commonly is time-consuming as well.

Alternatively, parameter estimation may be achieved by using nonlinear regression. Various methods for groundwater parameter estimation have been developed (e.g., Neuman and Yakowitz, 1979; Yeh, 1986; Cooley and Naff, 1990; Hill, 1992; Sun, 1996). We have been working with MODFLOWP (Hill, 1992) for estimation of parameters in a three-dimensional heterogeneous aquifer system by modeling aquifer test results using MODFLOW for the forward modeling. In addition to the utility programs for MODFLOW, we have developed several modifications to the MODFLOWP code to enhance usability. In particular, we have added changes to the code which:

1) simplify input by making all input to the program free format;
2) allow the user to easily change the number and combination of parameters for estimation in a given run by modifying one line rather than regenerating the whole .PAR file;

3) automatically calculate ROFFs, COFFs, and TOFFs for head observations;
4) print a message to the screen when estimated parameter values are outside the upper and lower limits; and
5) allow the user to monitor run time.

Each of the MODFLOWP utilities is discussed below with an example of its usage.

3.1. Free Format for Input of Data to the Parameter Estimation Package

With previous versions of MODFLOWP, all data input had to be entered according to highly structured formats. Data input to the .PAR file is complicated, and the formats vary between data sets in the file. To simplify data input to the .PAR file and reduce errors due to format problems, MODFLOWP has been modified to read the .PAR file as free format. Data sets still must follow the same line structure (i.e., same data elements on a given line, same sequence of lines and data sets) and use the same data types (i.e., integer, real) as before. However, data elements on a given line can be given in free format, and so they need only be separated by one or more spaces.

Structured format entry interprets blank spaces as zeros leading to a practice of not providing data for input values that are intended to have a value of zero. Free format requires zero values to be specified. Hence, all data values, including zero, must be supplied when using free format input.*

3.2. Enable Any Number and Combination of Parameters for Estimation

MODFLOWP input file format requires that parameters to be estimated should precede those that will remain unchanged. In Data Set 9 all positive group numbers need to precede any negative numbers (Hill, 1992). If the MODFLOWP user wishes to evaluate different combinations of parameters, the .PAR file has to be reorganized. Rebuilding the .PAR file can be time-consuming and may lead to input errors. The modified version of MODFLOWP presented here allows the user to choose any new or former combination of initially identified parameters in Data Set 9 for estimation without reorganizing the .PAR file. The user simply identifies in Data Set 9 those parameters that will *not* be evaluated by assigning negative group numbers to them. The negative numbers can be in any sequence.

3.3. Calculate and Enter Offsets inside MODFLOWP

MODFLOWP, as a numerical model, operates by discretizing time into time steps and space into grid cells with nodes in the centers of cells. Calculations of model results are made at time steps and nodes which generally do not correspond exactly with the time of observations or the locations of well screens. Such differences may not be significant in many modeling tasks, but they could add model error to the parameter estimation process and they may be significant for some modeling scenarios, especially for modeling of pumping test results at closely spaced partially penetrating wells in heterogeneous media.

MODFLOWP allows the user to specify offsets between locations of observation points and nodes setting the ROFF and COFF data values in the .PAR file, and between observation times and model time steps by setting TOFF values. The user must calculate each ROFF, COFF and TOFF outside of the code. These offsets must be recalculated and reentered each time the time or grid discretization are altered in subsequent model runs. Both activities can be time-consuming and error-

* If an F77 compiler is used, character input may need to be bracketed by apostrophes. For example in Example File 16, line 10, Q must be input as 'Q'.

prone. We have incorporated utilities into MODFLOWP which automatically calculate these offsets eliminating the need to enter them into the .PAR file.

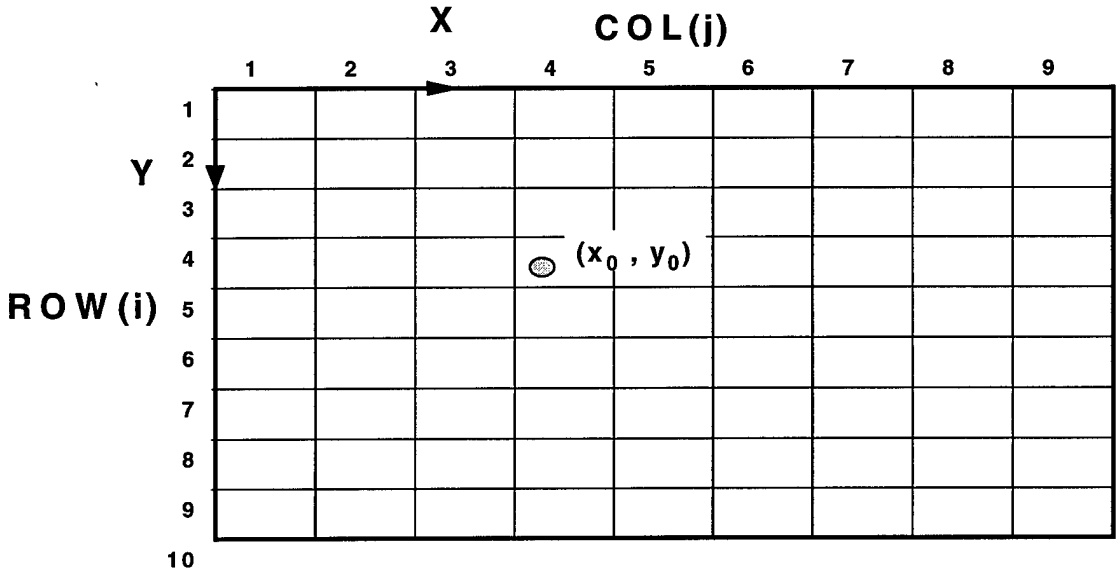


Figure 4. ROFF and COFF defined by absolute coordinates (x_0, y_0). Origin of x-y portion of coordinate system is in the upper left-hand corner of the model domain (the GMS default coordinate system).

3.3.1. Calculate and Enter ROFFs and COFFs

ROFFs and COFFs represent the offsets of an observation well from the center of the cell in row and column directions, respectively. They are used to calculate the head (or drawdown) for the observation well by interpolation of the calculated heads (or drawdown) of nearby cells. In MODFLOWP, ROFFs and COFFs have to be provided in Data Set 6 of the .PAR file. If grid discretization or locations of observation points are changed, ROFFs and COFFs have to be changed also.

Although the calculation of ROFFs and COFFs is not difficult (see MODFLOWP user's guide [Hill, 1992]), it is simpler to directly input the coordinates (x_0, y_0) of an observation well (Figure 4) and have the program calculate ROFFs and COFFs internally. That is, (x_0, y_0), the plane coordinates of an observation well are input, rather than ROFF and COFF and the row and column numbers of the well. There are at least two advantages with this input approach: (1) x, y coordinate locations are accurate and intuitive, and (2) ROFFs and COFFs will be automatically recalculated inside the program whenever the spatial discretization is changed.

3.3.2. Calculate and Enter TOFFs

TOFFs (time offsets) in MODFLOWP are used to calculate differences between actual observation times and the time steps used in the simulation. Standard MODFLOWP requires the user to input TOFFs and the corresponding time step in Data Set 6. Calculation and input for TOFFs are not difficult but can be time-consuming. Whenever temporal discretization is changed, the time steps

and TOFFs for Data Set 6 and Data Set 6C have to be changed.

Our modifications have made this task very simple: just input observation time t_i and observed head H_i, then the corresponding time steps and TOFFs are internally calculated within MODFLOWP. Advantages for direct input of t_i and H_i are: (1) users are most familiar with the measured head at a specific time making input errors easier to spot; (2) records of field measurements are usually time and head (or drawdown); thus the field records can be used directly with our modified input format and compared directly with the input file.

3.3.3. Input Instructions for Data Set 6

Corresponding with the modifications described above, the inputs for Data Set 6 and Data Set 6C need to be changed as follows:

Data Set 6: DID, NDER, X ,Y, OBST, HOBS, WT1, WT2, IWT, IPUT

- DID and NDER are the same as defined in the MODFLOWP user's guide.
- X and Y are the coordinates of an observation well.
- OBST is the time an observation was made. OBST $\geq$ 0 is the observation time if there is only one observation at this well. Otherwise OBST < 0 and the absolute value of OBST equals the number of observations at this well, and OBST must be entered as a real number. For example, if three observations are made, OBST = -3.0.
- Definitions for HOBS, WT1, WT2 and IWT are the same as in the MODFLOWP user's guide.
- IPUT is a new flag defined in this report indicating whether the same weights (IPUT = 0) will be used for all observations at this well, or if different weights (IPUT > 0) will be specified.

Data Set 6C: DID, OTIME, HOBS, WT1, WT2, IWT

- DID is the same as defined in the MODFLOWP user's guide.
- OTIME is the observation time. This replaces time step and time offset in Data Set 6C
- Definitions for HOBS, WT1, WT2 and IWT are the same as in the MODFLOWP guide.

3.4. Announce Parameter Values out of Upper and Lower Limit Bounds

In MODFLOWP, parameter bounds are only used for reference in the output file and are not used in the regression solution. Estimated parameters may be outside the bounds of expected, reasonable, bounds. For example, during a MODFLOWP run specific yield, S_y, may be estimated to be larger than 0.5; specific storage, Ss, may become zero; K for a sand layer may have an estimated value that is lower than that of a shale.

To identify parameter estimation runs that are in progress, but not likely to result in a meaningful set of parameter estimates, a message will be sent to standard output (screen) if any evaluated parameter is set beyond one of the bounds specified in Data Sets 8A and 8B. The message identifies the parameter, the parameter value, and the parameter limit violated. This allows the modeler to terminate the MODFLOWP run, which may take hours or days to complete, when it is

obvious the program is not converging on a reasonable solution. A message will also be printed if the value of a parameter changes sign during an estimation run.

3.5. Monitor Run Time

As mentioned above, a given parameter estimation run may take a long time because of the number of parameters being estimated, the complexity of the hydrological processes being modeled, and the nonlinear nature of the problem. For the modeler, feedback on the amount of CPU time used for a given iteration is sometimes a useful indication of whether the investigated problem is "moderately" or "highly" nonlinear, because a highly nonlinear problem usually takes a longer time to converge. The modified program prints to file and writes out to the screen the elapsed run time since the starting date and time for each iteration.

Monitoring the run time requires the use of non-standard FORTRAN routines. We have supplied seven versions of the run time routines. The following table lists file names to be used for specific compilers:

time_f90.for	FORTRAN 90
time_g77.for	GNU g77 FORTRAN
time_ms.for	Microsoft Power Station FORTRAN
time_duf.for	Digital FORTRAN for UNIX
time_sun.for	Sun FORTRAN
time_sgi.for	SGI FORTRAN
time_dum.for	Disables time calls for use with any compiler

The list of compiler coverage is far from exhaustive. However, many compilers adhere to non-FORTRAN standards. Hence, the coding is more generally applicable than listed here. The routine time_f90.for uses the FORTRAN 90 standard time calls which are supported by a large number of FORTRAN 77 and FORTRAN 90 compilers. Using time_dum.for removes time monitoring from the program without requiring modification of the source code. The file time_dum.for can be used with any compiler because it simply returns to the call statement without executing the timing routines.

3.6. Example .PAR and Output Files

The following example is taken from Test Example 1 of the MODFLOWP user's guide (Hill, 1992), but is changed for use with the modified version of MODFLOWP presented with this report. Consider the sequence of modeling runs where initially 9 parameters are estimated using the observed drawdown from several wells. In our test of the modified MODFLOWP program, we start with the same input sequence of 9 parameters but now we just want to estimate 7 of them: in sequence positions 2, 4, 5, 6, 7, 8, and 9. To evaluate parameters in sequence positions 2, 4, 5, 6, 7, 8, and 9 only, the user changes the sign in Data Set 9 for the group numbers of those parameters that will NOT be estimated: -3, 4, -5, 6, 3, 4, 7, 7, 1 (Example File 16). In Example File 16, Comments lines starting with @@@ have been added to the .PAR file listing to highlight the changes made to the .PAR file for Test Example 1. In addition to the modification of Data Set 9, observation well drawdown data and the pumping well drawdown data, Data Set 6C, has been input with free format.

The affected portions of the corresponding output file are given in Example File 17.

Example File 16. Annotated (@@@) portions of the MODFLOWP .PAR file.

```
TWO-LAYER EXAMPLE - TRANSIENT                                                    LINE 1
Modified Test Case 1 of Hill (1992,Appendix A)                                   LINE 2
    9    5   56    4    2    3    0    1                                        LINE 3
    2    1    1                                                                 LINE 4
   32    0    0    1   18    3    0    0                                        LINE 5
    1   -1    1    0    0                                                       LINE 6
   40   33    0    0    0    0    0    0    0    0    0    0    0               LINE 7
@@@ All zero values must be included
    1    0    0    0                                                           LINE 8
   30                                                                          DATA SET 1A
Q   0   -2    1   15   -1 0                                                    DATA SET 2
         1.        0
          1         9        10       1.0                                     DATA SET 2A
          2         9        10       1.0
S1  1   -1    0    0    0    0                                                 DATA SET 2
@@@ All zero values must be included
                      ⋮

1.0      1    500.    2500.   -3.0    0.00    1.0025    0.0025    0    0      DATA SET 6
@@@ Input x and y coordinates.  Number of observations is real value

   2                                                                           DATA SET 6B
1.0      0.00        101.804                                                   DATA SET 6C
@@@ Input observation time not time step and offset
@@@ Observation weighting taken from Data Set 6

1.1      87162.0     101.775
1.12    24439068.0   101.675
                      ⋮

6.0      2     3500.0   3500.0      -3.0    0.0  0.000  0.000    0   1       DATA SET 6
@@@ transient observation weight option set to 1

   2                                                                           DATA SET 6B
6.0        0.00   126.537  1.0025  0.0025    0                               DATA SET 6C
@@@ Full control of weighting for each observation

6.1     87162.0  126.542  1.0025  0.0025    0
6.12 24439068.0   112.172  1.0025  0.0025    0
                      ⋮
         -1.074     1.38E-3      .426E-03       1.2E-3        1.E-7        2.E-4
       4.0E-5       2.E-8        1.0E-8                                    DATA SET 8
         -0.8       1.3E-2       3.00E-3       1.2E-2        1.E-6        2.E-3
       4.0E-4       2.E-7        1.0E-7                                    DATA SET 8A
         -1.4       1.3E-4       3.00E-5       1.2E-4        1.E-8        2.E-5
       4.0E-6       2.E-9        1.0E-9                                    DATA SET 8B
          -3           4            -5            6             3            4
           7           7             1                                     DATA SET 9
@@@ inactive parameters may be interspersed with active parameters
```

Example File 17. Annotated (@@@) portions of the MODFLOWP output file.

```
1                                MODFLOW
  U.S. GEOLOGICAL SURVEY MODULAR FINITE-DIFFERENCE GROUND-WATER FLOW MODEL - MODFLOWP
 BSU August, 1998 Modified Version          @@@ Announcement of special version
 See Boise State University Technical Report BSU CGISS 97-02
                    ⋮
 OBSERVED HEAD DATA
```

@@@ Observation time or number of transient observations as item 6.

```
   OBS#   ID    LAYER ROW COLUMN    OBS. TIME   TIME STEP ROW/COLUMN/TIME OFFSETS OBS. HEAD STATISTIC
     1  1.0      1     3     1       -3.000       -3        .000     .000     .000     .000        1.00250
  TRANSIENT DATA AT THIS LOCATION, ITT =    2
     1  1.0                          .000        0              .000      101.80      1.0025
     2  1.1                       87162.000      1              .000     -.28999E-01  .25000E-02
     3  1.12                   24439070.000     12              .000     -.12900      .25000E-02
```

@@@ Observation time and time step and offset listed.

```
 PARAMETER INFORMATION:
  (CONVERGENCE CRITERIA LISTED HERE ARE USED TO SOLVE FOR SENSITIVITY-EQUATION SENSITIVITIES)
     #  ID  INITIAL VALUE  LN        UPPER VALUE  LOWER VALUE  CONVERGENCE CRITERIA   GROUP#  WEIGHT
OF PRIOR EST.
     2  S1       .1380E-02  1       .1300E-01     .1300E-03     .725E-02     .000        4
     4  KST      .1200E-02  1       .1200E-01     .1200E-03     .833E-02     .000        6
     5  KV       .1000E-06  1       .1000E-05     .1000E-07     100.         .000        3
     6  S1       .2000E-03  1       .2000E-02     .2000E-04     .500E-01     .000        4
     7  T        .4000E-04  1       .4000E-03     .4000E-05     .250         .000        7
     8  RCH      .2000E-07  0       .2000E-06     .2000E-08     500.         .000        7
     9  RCH      .1000E-07  0       .1000E-06     .1000E-08     .100E+04     .000        1
     1  Q       -1.074      0      -.8000        -1.400         .000         .000       -3
     3  T        .4260E-03  0       .3000E-02     .3000E-04     .000         .000       -5
```

@@@ inactive parameters listed last.

```
 SCALED SENSITIVITIES (SCALED BY B*(WT**.5))

 PARAMETER # :        2          4          5          6          7          8          9
 PARAMETER ID :       S1         KST        KV         S1         T          RCH        RCH
 OBS# & ID
    1  1.0          .000       1.51      -.445E-07  .000      -.228E-04  .150       .749E-01
    2  1.1         -.123E-01 -.397E-02 -.113E-02 -.359E-02  .621E-02  .800E-06  .400E-06

       COMPOSITE SCALED SENSITIVITIES:
       ((SUM OF THE SQUARED VALUES)/ND)**.5
                  235.       25.7       123.       57.7       498.       11.9       11.0
```

Run time [min]: .1500 since 8/12, 11:24

@@@ Run time of first iteration.

```
 ITERATION NO. =     1
 VALUES FROM LEAST-SQUARES REGRESSION PROCEDURE :
   DET OF SCALED LEAST-SQUARES MATRIX =  .25575E-02
   MARQUARDT PARAMETER (AMP)--------- =  .00000
   FACTOR FOR SCALING PAR. CHANGE (AP)=  1.0000
   MAX. FRACTIONAL PAR. CHANGE (DMX)  =  .76297
   MAX. FRAC. CHANGE OCCURRED FOR PAR.#      5

 UPDATED ESTIMATES OF REGRESSION PARAMETERS :
     S1           KST          KV           S1           T            RCH          RCH
 PAR.#    2            4            5            6            7            8            9
0  .11753E-02   .11331E-02   .17630E-06   .10834E-03   .49218E-04   .11507E-07   .15596E-07
```

Run time [min]: .2167 since 8/12, 11:24

@@@ Cumulative run time at each iteration.

```
 ITERATION NO. =     2

 PARAMETER SUMMARY
 ------------------

 PARAMETER # :        2          4          5          6          7          8          9
 PARAMETER ID :       S1         KST        KV         S1         T          RCH        RCH
 FINAL VALUES
                  -.677E+01 -.682E+01 -.153E+02 -.988E+01 -.994E+01  .109E-07  .160E-07
   EXPONENTIAL OF LN PARAMETERS
   (0.0 FOR UNTRANSFORMED PARAMETERS)
                   .115E-02  .109E-02  .222E-06  .512E-04  .481E-04  .000E+00  .000E+00
 STD. DEV.
                   .387E-01  .797E-01  .782E-01  .706E+00  .513E-02  .128E-08  .680E-09
 COEF. OF VAR.
                   .572E-02  .117E-01  .510E-02  .715E-01  .516E-03  .118E+00  .426E-01

 UPPER LIMIT, LINEAR 95-PERCENT CONF. INT.
                  -.669E+01 -.666E+01 -.152E+02 -.847E+01 -.993E+01  .134E-07  .173E-07
   EXPONENTIAL OF LN PARAMETERS
```

```
  (0.0 FOR UNTRANSFORMED PARAMETERS)
                .125E-02  .128E-02  .259E-06  .210E-03  .486E-04  .000E+00  .000E+00

LOWER LIMIT, LINEAR 95-PERCENT CONF. INT.
               -.684E+01 -.698E+01 -.155E+02 -.113E+02 -.995E+01  .830E-08  .146E-07
  EXPONENTIAL OF LN PARAMETERS
  (0.0 FOR UNTRANSFORMED PARAMETERS)
                .107E-02  .932E-03  .190E-06  .125E-04  .476E-04  .000E+00  .000E+00
                    :
Run time [min]:       .4500 since  8/12, 11:25
```

@@@ Total run time used.

4. OBTAINING SOURCE CODE

Source code of our modifications is available under the listing for this report at http://kihei.idbsu.edu/cgiss_pub.html. Compacted archives in both WINZIP® and tar formats are available which include a modified source code for both MODFLOW and MODFLOWP, example input and output files, and UNIX 'diff' files which highlight the changes made to the MODFLOW and MODFLOWP programs. To obtain a copy of these archives connect to http://kihei.idbsu.edu/cgiss_pub.html with a web-browser, follow the Technical Report Publications link, and then scroll to Huang et al.. The report listing has been set up as a link to downloading instructions for the source code archive files.

5. SUMMARY

This report serves as documentation and user's guide for (1) a number of stand-alone utilities to assist with input to MODFLOW and (2) code modifications internal to MODFLOW and MODFLOWP. These were developed to improve efficiency of use of MODFLOW and MODFLOWP for modeling groundwater flow in three-dimensional heterogeneous systems. Several utilities to assist with input to MODFLOW are specifically designed for use with the pre- and post-processor package: Groundwater Modeling System (GMS) and are identified as such in this report. New features for MODFLOW include routines for:

1) assignment of material blocks and material types to these blocks within a given three-dimensional grid mesh;
2) distribution of pumping rate for individual model layers for a well that draws from or injects into multiple layers;
3) calculation of weighted drawdown for an observation well screened over multiple layers; and
4) customizing the drawdown output file to contain data for a specified number of observation wells (rather than for all nodes individually).

For MODFLOWP, the program has been modified to:

1) simplify input by making all input to the program free format;
2) allow the user to easily change the number and combination of parameters for estimation in a given run by modifying one line rather than regenerating the whole .PAR file;
3) automatically calculate ROFFs, COFFs, and TOFFs;
4)announce parameter estimates outside the upper or lower limits during program execution; and
5) allow the user to monitor run time.

6. ACKNOWLEDGMENTS

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