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MODFLOW-2000, THE U.S. GEOLOGICAL SURVEY MODULAR GROUND-WATER MODEL — DOCUMENTATION OF EFFECTIVE-POROSITY PARAMETERS IN THE ADVECTIVE-TRANSPORT OBSERVATION (ADV2) PACKAGE

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PREFACE

The computer software described in this report is a new capability of the Advective-Transport Observation (ADV2) Package for MODFLOW-2000, the U.S. Geological Survey's three-dimensional ground-water flow parameter-estimation model. The software is designed to allow effective porosity, which is used to calculate seepage velocity from specific discharge, to be defined as a parameter in the ADV2 Package. Sensitivity-equation sensitivities can be calculated for defined effective-porosity parameters. These sensitivities can be used for sensitivity analysis, sampling strategy, parameter estimation, and uncertainty evaluations. The documentation presented here describes the methods used, the modifications to the ADV2 input file, and the output related to the new effective-porosity parameters. The resulting ADV2 Package is fully backward compatible with previous versions.

All code developed by the U.S. Geological Survey for MODFLOW-2000 is available for downloading over the Internet from a U.S. Geological Survey software repository. The repository is accessible on the World Wide Web from the U.S. Geological Survey Water Resources Information web page at URL http://water.usgs.gov/software/ground_water.html, at the entry labeled 'MODFLOW-2000'.

The performance of the effective-porosity parameters of the ADV2 Package has been tested in a variety of applications. Future applications, however, might reveal errors that were not detected in the test simulations. Users are requested to notify the U.S. Geological Survey of any errors found in this document or the computer program using the email address available on the website mentioned above. Updates might occasionally be made to both this document and to the effective-porosity parameters of the ADV2 Package, and users are encouraged to check the website periodically.

Revised, 2005

The term 'Darcy velocity' is replaced by 'seepage velocity' and 'Darcy flux' is replaced by 'specific discharge' to conform to terminology suggested by Zheng and Bennett (2002). We thank Leonard F. Konikow of the U.S. Geological Survey who made us aware of our incorrect terminology.

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DOCUMENTATION OF EFFECTIVE-POROSITY PARAMETERS IN THE ADVECTIVE-TRANSPORT OBSERVATION (ADV2) PACKAGE

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Abstract

This report documents the effective-porosity parameters for model layers and confining units (parameter types PRST and PRCB, respectively) of the Advective-Transport Observation (ADV2) Package (Anderman and Hill, 2001) of MODFLOW-2000 (Harbaugh and others, 2000; Hill and others, 2000). Effective-porosity parameters are used to calculate seepage velocity from specific discharge. Sensitivity-equation sensitivities can be calculated for defined effective-porosity parameters. These sensitivities can be used for sensitivity analysis, parameter estimation, and uncertainty evaluations. Of simulated quantities calculated by the Observation Process of MODFLOW-2000 (for example hydraulic head or flows at head-dependent boundaries), only advective transport simulated using ADV2 are sensitive to the effective-porosity parameters.

Introduction

Ground-water models calculate specific discharges. To simulate advective transport through a ground-water system, these specific discharges need to be converted to seepage velocities by dividing by local values of effective porosity.

Previous versions of the Advective-Transport Observation (ADV2) Package have not allowed the use of parameters to define effective porosity of model cells and confining beds. As a result, effective porosity could not be formally considered in sensitivity analyses, could not be estimated using the Parameter-Estimation Process of MODFLOW-2000, and could not be considered when evaluating the uncertainty of predicted advective transport. The capability documented in this work alleviates these limitations.

This report first describes how effective porosity is used to calculate the Darcian velocity of a particle. For most readers, this section and Appendix A, which documents the input and output of the new capability, are likely to be the most used part of this report.

Appendix B of this report presents the equations used to change the Ground-Water Flow Process and the Sensitivity Process of the MODFLOW Advective-Transport Observation Package. This appendix is likely to be of interest to readers concerned with how the capability was programmed.

Using Effective Porosity to Calculate Cell-Face Velocities

Like most numerical ground-water models, when using MODFLOW-2000 the system is discretized into relatively small, distinct volumes and the model calculates the amount of water that flows through these volumes. In MODFLOW-2000 these volumes are called finite-difference cells, and each has six faces as shown in Figure 1. For each finite-difference cell, the model calculates the amount of water flowing through each of the six cell faces.

For each cell face, the flow through it can be divided by the area of the cell face. The result is called the cell-face specific discharge, which is the flow per unit area of the cell face. The specific discharge is not the rate of flow experienced by fluid particles or solutes they carry because the cell face is partially occupied by geologic material through which water cannot flow, such as sand. Over the cell area, the average rate of flow experienced by fluid particles and the solutes they carry is called the seepage velocity. The seepage velocity can be calculated by dividing the cell-face flow by the area of the cell face available to flow. Equivalently, the seepage velocity can be calculated as the specific discharge divided by the effective porosity of the geologic material. Effective porosity is discussed and typical values provided in a number of texts, including Zheng and Bennett (2002).
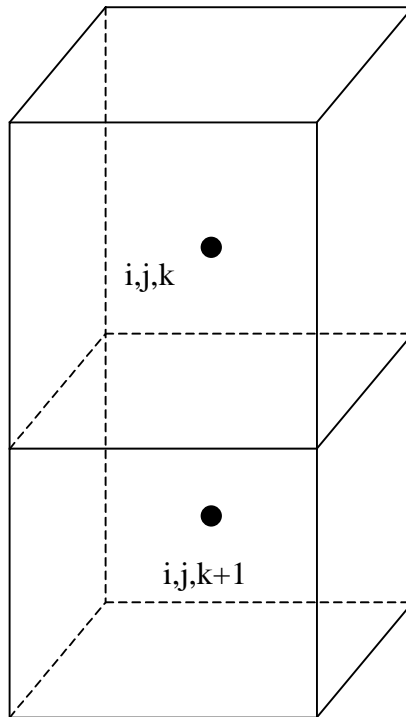
Figure 1: A finite difference cell associated with the node at row i, column j, and layer k, with the cell below shown. Most cells would also have adjoining cells on the four sides and the top.

Effective Porosity Parameters

A value of effective porosity needs to be assigned to every finite-difference cell in the grid, but these values may not be independent of one another. Often it is convenient to define a limited number of parameters that are used to define the cell values. Using this updated version of ADV2 , parameters can be used as described by Harbaugh and others (2000, p. 12-19) to define the distribution of effective porosity. The methods for specifying parameters are very general and are the same as used for other parts of MODFLOW-2000. They include multiplication and zone arrays, so that spatial variations can be smooth or abrupt. Also, the parameters can be additive, which allows most interpolation methods, such as kriging, to be used.

By specifying the distribution of effective porosity using parameters in MODFLOW-2000, the Sensitivity and Parameter-Estimation Processes of MODFLOW-2000 can be used to address questions such as what observations might assist in estimating the effective-porosity parameter values, whether an existing set of observations offer any information of effective porosity, what values of effective porosity would produce the best fit to a set of observations, whether effective porosity is important to predictions of interest, and how uncertainty in the

estimated effective porosity affects uncertainty in the predictions. Methods and guidelines for approaching these and other questions are presented by Hill (1998).

Effective Porosity Sensitivities

The effective porosity sensitivities are calculated analytically as described in Appendix B. Conceptually, they can be thought of as the amount a simulated value will change given a small change in the value of a parameter used to define the effective-porosity distribution. These sensitivities are used to address the questions posed in the paragraph above.

References Cited

Anderman, E.R. and Hill, M.C., 2001, MODFLOW-2000, The U.S. Geological Survey Modular Ground-Water Model — Documentation Of The Advective-Transport Observation (ADV2) Package, Version 2: U.S. Geological Survey Open-File Report 01-54, 69 p. , accessed September 4, 2003 at http://water.usgs.gov/nrp/gwsoftware/modflow2000/modflow2000.html

Harbaugh, A.W., Banta, E.R., Hill, M.C., and McDonald, M.G., 2000, MODFLOW-2000, the U.S. Geological Survey modular ground-water model, User's guide to the Modularization concepts and the Ground-Water Flow Process: U.S. Geological Survey Open-File Report 00-92, 121 p. , accessed September 4, 2003 at http://water.usgs.gov/nrp/gwsoftware/modflow2000/modflow2000.html

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Zheng, Chunmaio, and Bennett, G.D., 2002, Applied contaminant transport modeling, second edition: New York, John Wiley, 621p.

Appendix A: Effective-Porosity Parameter Input and Output

Changes to the ADV2 Input Instructions

The ADV2 input instructions are presented by Anderman and Hill (2001, p. 48-53). Here, the changes to the input file required to define effective-porosity parameters are presented.

To allow the definition of effective-porosity parameters, item 2 of the ADV2 Package input file can be different than described by Anderman and Hill (2001, p. 49). If parameters are to be defined, Item 2 needs to start with the word "PARAMETER" and have the following form:

```
2.   'PARAMETER' NPADV IPFLG
2a. [PARNAM PARTYP Parval NCLU]
2b. [Layer Mltarr Zonarr IZ]
```

Each repetition of Item 2b is called a parameter cluster. Repeat Item 2b NCLU times.

Repeat Items 2a-2b for each parameter to be defined (that is, NPADV times).

The capability to define some porosity values using parameters and others without using parameters is not provided. Thus, if parameters are used to define the porosity, then they must define porosity for all model cells and Quasi-3D confining beds. Conversely, if the prior method of defining porosity using layer arrays is used, then no porosity parameters can be defined.

Explanation of Variables Read by the ADV2 Package

NPADV – is the number of ADV parameters, which equals the number of effective-porosity parameters.

IPFLG – is the print code for all ADV parameters, which controls the printing of the porosity arrays created when the parameters are substituted into the arrays.

PARNAM – is the name of a parameter to be defined. This name can consist of up to 10 characters and is not case sensitive.

PARTYP – is the type of parameter to be defined. For the ADV2 Package, the supported parameter types are:

PRST – defines the effective porosity of the material represented by a model layer.

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PRCB – defines the effective porosity of the material represented by a quasi-3D confining unit.

Parval – is the parameter value. This parameter value may be overridden by a value in the Sensitivity Process input file or by a value generated by the Parameter-Estimation process.

NCLU – is the number of clusters required to define the parameter. Each repetition of item 2b is called a cluster, with variables Layer, Mltarr, Zonarr, and IZ.

Layer – is the model-layer number to which a cluster definition applies. Even if the Hydrogeologic-Unit Flow Package (Anderman and Hill, 2001) is used, the effective porosity is defined by model layer, not hydrogeologic unit.

Mltarr – is the name of the multiplier array to be used to define array values that are associated with a parameter. The name "NONE" means that there is no multiplier array, and the array values will be set equal to Parval.

Zonarr – is the name of the zone array to be used to define array elements that are associated with a parameter. The name "ALL" means that there is no zone array and that all elements in the model layer are part of the parameter.

IZ – is up to 10 zone numbers (separated by spaces) that define the array elements that are associated with a parameter. These values are not used if Zonarr is specified as "ALL". Values can be positive or negative, but 0 is not allowed. The first zero or non-numeric value terminates the list.

Example ADV2 input file

The following ADV2 input file is an example of the file used for Test Case 1 of the ADV2 documentation, with effective porosity defined using one parameter with parameter name Porosity1. The lines used to define the effective-porosity parameter are in bold type.

```
   1   1   00   1   1   0      0.    0                                 ITEM 1
PARAMETER  1    2                                                      ITEM 2
Porosity1  PRST  1.0  1                                                ITEM 2a
1  PRST_Mult  ALL                                                      ITEM 2b
   1   1   12   16  0.0  0.0  0.0                                      ITEM 3
B_1     1   15   20  0.0 0.4621 -0.3815 500.  1 500.  1  1.  1  13879.5 3   ITEM 4
  0                                                                    ITEM 5
```

Appendix B: Program Changes

Changes to the MODFLOW Ground-Water Flow Process

Particle displacement depends on the effective porosity of the geologic material though the calculation of the Darcian velocity. In the Layer-Property Flow (LPF) and the Hydrogeologic-Unit Flow (HUF) Packages, one of which would be used for any single simulation, effective-porosity parameters can be defined for model layers. In the LPF Package, effective porosity also can be defined for quasi-three-dimensional confining units. These are described in the following sections

Model Layers – Parameter type PRST

The velocity on the left x-face of cell *i,j,k* is defined as the flow rate through the cell face divided by the effective area of flow as given by equation B-9 of Anderman and Hill (2001, p. 61):

$$v_{x_{i,j-1/2,k}} = \frac{2Q_{x_{i,j-1/2,k}}}{n_{i,j,k}\Delta c_i \left(l_{i,j-1,k} + l_{i,j,k} \right)}$$ (B-1)

where

$v_{x_{i,j-1/2,k}}$ is the velocity on face *i,j-½,k* [L/T],

$Q_{x_{i,j-1/2,k}}$ is the cell-face flow rate [L^3/T],

$n_{i,j,k}$ is the effective porosity of cell *i,j,k*,

Δc_i is the cell width of row i [L],

$l_{i,j,k}$ is the saturated thickness of unconfined cell *i,j,k* or thickness of confined cell
       i,j,k [L].

In this work, the effective porosity can be defined using parameters, so that

$$n_{i,j,k} = \sum_{l=1}^{p} n_l m_{l_{i,j,g}}$$ (B-2)

where,

p is the number of additive parameters that define the effective porosity,

n_l is the value of parameter *l*, and

$m_{l_{i,j,k}}$ is the multiplication factor for parameter *l* at model grid row *i*, column *j*, and

model layer *k*

The cell-face velocities of equation 1 are calculated using an average saturated thickness, instead of the single-cell saturated thickness used in MODPATH, because the original method produces discontinuities in velocity, and thus in sensitivity, at cell boundaries.

The above derivation is for the x-component of flow. Similar equations can be derived in the y direction.

Vertical velocity is calculated from the flow between layers by dividing the vertical flow by the effective area of flow using Equation B19 of Anderman and Hill (2001). If the particle is between the centers of model layers k and $k+1$ and in model layer k, the velocity is:

$$v(k)_{z_{i,j,k+1/2}} = \frac{Q_{z_{i,j,k+1/2}}}{n_{i,j,k}\Delta r_j \Delta c_i} \qquad \text{(B-3a)}$$

and if the particle is in model layer $k+1$ the velocity is:

$$v(k+1)_{z_{i,j,k+1/2}} = \frac{Q_{z_{i,j,k+1/2}}}{n_{i,j,k+1}\Delta r_j \Delta c_i} \qquad \text{(B-3b)}$$

The capability documented by this work allows the effective porosity to be represented using parameters as shown in equation 2.

Quasi-Three-Dimensional Confining Layers – Parameter Type PRCB

When using the Layer-Property Flow Package (Harbaugh and others, 2000, p. 29-31), flow through quasi-three-dimensional confining units is assumed to be vertical. In this case, the velocity is calculated using equation B-21 of Anderman and Hill (2001, p. 66) as:

$$v_{z_{i,j,c}} = \frac{Q_{z_{i,j,k+1/2}}}{n_{i,j,c}\Delta r_j \Delta c_i} \qquad \text{(B-4)}$$

where

$n_{i,j,c}$ is the effective porosity of the confining bed in column j of row i.

Using the ADV2 Package as modified for this work, the effective porosity can be defined using parameters, so that

$$n_{i,j,c} = \sum_{l=1}^{p} n_l m_{l_{i,j,c}} \qquad \text{(B-5)}$$

which is equivalent to equation B-2 except that the subscript c is used instead the k because here quasi-three-dimensional layer c is identified.

Contribution to the MODFLOW Sensitivity Process

The sensitivity of velocity within a model layer with respect to effective porosity is obtained by taking the partial derivative of equations B-1 through B-5 with respect to an effective-porosity parameter n_l. Using equation B-1 yields:

$$\frac{\partial v_{x_{i,j-1/2,k}}}{\partial n_l} = \frac{-2Q_{x_{i,j-1/2,k}}}{n_{i,j,k}^2 \Delta c_i \left(l_{i,j-1,k} + l_{i,j,k} \right)} = -\frac{v_{x_{i,j-1/2,k}} m_{l_{i,j,g}}}{n_{i,j,k}} \tag{B-4}$$

The expression is not more complicated because the cell-face flow rate does not depend on effective porosity.