

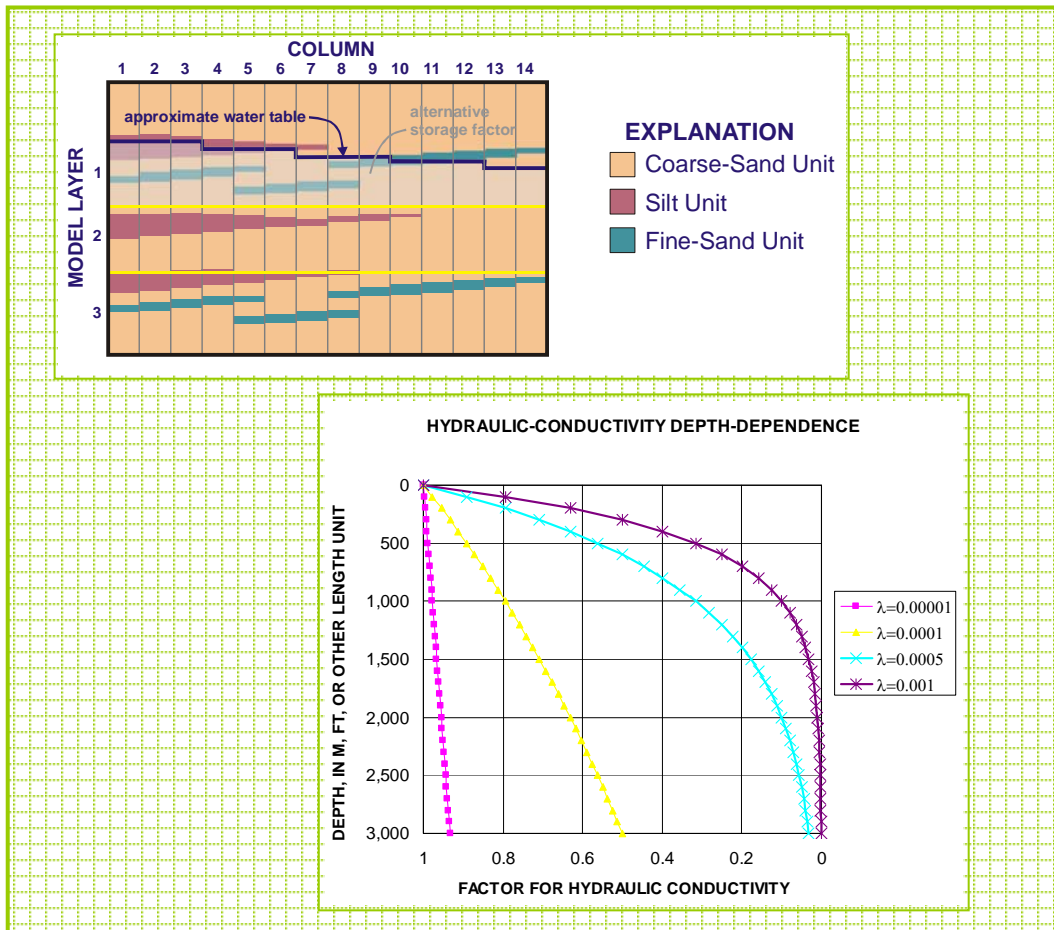


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U.S. Department of Energy

MODFLOW-2000, THE U.S. GEOLOGICAL SURVEY MODULAR GROUND-WATER MODEL — THREE ADDITIONS TO THE HYDROGEOLOGIC-UNIT FLOW (HUF) PACKAGE:

- ALTERNATIVE STORAGE FOR THE UPPERMOST ACTIVE CELLS (SYTP PARAMETER TYPE),
- FLOWS IN HYDROGEOLOGIC UNITS, AND
- THE HYDRAULIC-CONDUCTIVITY DEPTH-DEPENDENCE (KDEP) CAPABILITY

Open-File Report 03-347



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By Evan R. Anderman¹, and Mary C. Hill²

U.S. Geological Survey

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¹ Calibra Consulting LLC, Denver, CO, USA

² U.S. Geological Survey, Boulder, CO, USA

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For additional information write to:

Regional Research Hydrologist
U.S. Geological Survey
Box 25046, Mail Stop 413
Denver Federal Center
Denver, CO 80225-0046

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PREFACE

The computer software described in this report adds three new capabilities to the Hydrogeologic-Unit Flow (HUF) Package for MODFLOW-2000, the U.S. Geological Survey's three-dimensional ground-water flow, sensitivity-equation sensitivity, and parameter-estimation model. The documentation presented here describes the methods used, and the new input and output.

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.

The performance of the new capabilities of the HUF 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 HUF Package, and users are encouraged to check the website periodically.

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ABSTRACT

The Hydrogeologic-Unit Flow (HUF) Package is an internal flow package for MODFLOW-2000 that allows the vertical geometry of the system hydrogeology to be defined differently than the definition of model layers. Effective hydraulic properties for the model layers are calculated using the hydraulic properties of the hydrogeologic units. The HUF Package can be used instead of the Block-Centered Flow (BCF) or the Layer Property Flow (LPF) Packages. This report documents three additions to the HUF Package.

Alternative specification of storage properties for the uppermost active cells.

Simulating the water table in a ground-water model as a free surface can be problematic because of nonlinearities that cause solver instabilities. These instabilities can be tempered in many situations by making the top of the system confined and assigning the storage coefficient to equal the specific yield. In the Hydrogeologic-Unit Flow Package, however, this can be difficult because storage properties are assigned using hydrogeologic units, not model layers. A new parameter type called SYTP addresses this difficulty by assigning an alternative storage property to the uppermost active model cells.

Calculation of flows in hydrogeologic units. The HUF Package was modified to calculate flows in hydrogeologic units. With these modifications hydrogeologic-unit water budgets can be computed and hydrogeologic units are accounted for when tracking particles with the Advective-Transport Observation (ADV) Package (Anderman and Hill, 2001).

Hydraulic-Conductivity Depth-Dependence (KDEP) Capability. The HUF package also was modified to allow the horizontal hydraulic conductivity of hydrogeologic units to vary with depth using an exponential decay function. The vertical hydraulic conductivity changes

accordingly if specified using vertical-anisotropy (VANI) parameters. The surface elevation used to determine the exponential decay can be the top of the first model layer or another surface.

INTRODUCTION

The Hydrogeologic-Unit Flow (HUF) Package is an internal flow package for MODFLOW-2000 that can be used instead of the Block-Centered Flow (BCF) or the Layer Property Flow (LPF) Package. The HUF Package allows the vertical geometry of hydrogeologic units to be defined differently than the definition of model layers. An example of this capability is shown in Figure 1. Hydrogeologic units may be coincident with model layers, or they may be quite different. Unlike model layers, hydrogeologic units may pinch out. There may be multiple hydrogeologic units within a model layer, or many model layers may occupy the thickness of a hydrogeologic unit.

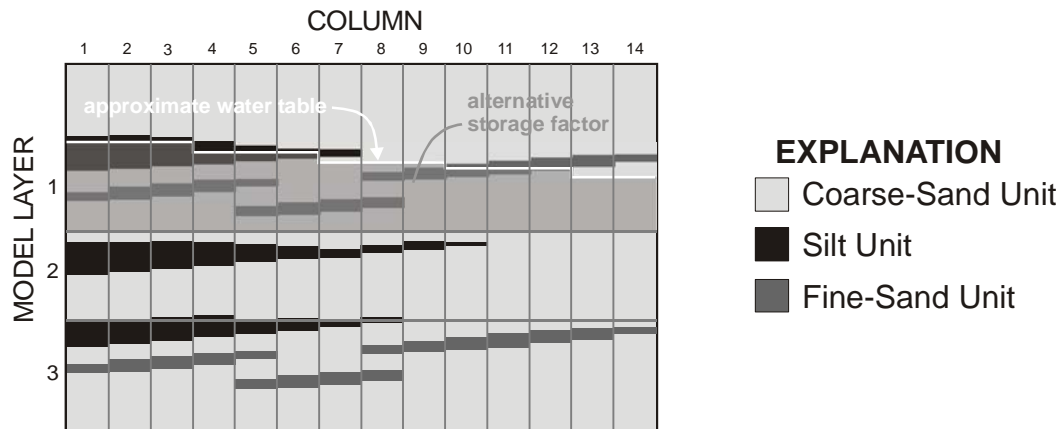


Figure 1: Hydrogeologic units composed of coarse sand, silt, and fine sand simulated with three model layers.

The three additions presented in this work substantially enhance the functionality of the HUF Package. These additions include a storage alternative for the upper most active model cells, a utility to compute flow through hydrogeologic units, and the hydraulic conductivity depth-dependence capability.

Purpose and Scope

The purpose of this report is to document three new additions to the HUF Package: (1) alternative storage for the uppermost active cell, (2) calculation of flows in hydrogeologic units, and (3) the hydraulic-conductivity depth-dependence (KDDEP) capability. The following sections describe the new capabilities in detail. The modified HUF Package input file is presented in Appendix A. Input instructions, model output, and program modifications for the hydraulic conductivity depth-dependence capability are presented in Appendix B.

Acknowledgements

The authors acknowledge Rick Waddell and Debra Cave of HSI-Geotrans, Inc. for their encouragement to include the depth-dependence capability in the HUF Package.

ALTERNATE STORAGE SPECIFICATION FOR THE UPPERMOST ACTIVE MODEL CELLS (SYTP)

Simulating the water table in a ground-water model as a free surface can be problematic. The problem occurs partly because the water-table elevation depends on the hydraulic conductivity of the water-table aquifer multiplied by the aquifer's saturated thickness. However, the saturated thickness depends on the unknown water-table altitude. This non-linearity often creates solver instabilities and can result in long execution times, particularly for transient, parameter-estimation simulations.

Nonlinearity due to water-table conditions can be managed by making the top model layer confined with a top elevation equal to the approximate elevation of the water table, as suggested by Hill (1998, p. 31) and Hill and others (2000, p. 25). This method is very useful during model calibration when in early runs simulated hydraulic heads may be greatly in error. The difficulty in using this method with the HUF Package is that it is not always clear what hydrogeologic units intersect the approximate water table used to define the top of the system. In this section a new parameter type called SYTP is introduced to address this difficulty. When one or more SYTP parameters are defined and all model layers are confined, the top active cell in each row, column location is assigned a specific yield using the SYTP parameters.

Modified Input Instructions

Storage-alternative parameters are defined using repetitions of Items 10 and 11, called parameter clusters, in the HUF Package. Parameter clusters for storage-alternative parameters work the same as for other parameter types with the exception that only one parameter cluster is needed for each parameter (that is, in item 10 NCLU = 1 and there needs to be only one Item 11). Both the second variable for item 10 (PARTYP) and the first variable for the corresponding item 11 (HGUNAM) need to be set to "SYTP". The modified HUF Package input file listed in Appendix A includes these changes.

Program Changes

Support for storage-alternative parameters is implemented in both the Ground-Water Flow Process and the Sensitivity Process, as described in the following sections. Even when listed, the SYTP parameter type is only used when *all* layers are confined. If any model layer is convertible, the SYTP parameters are ignored.

Ground-Water Flow Process

The storage-alternative parameter is used to replace the primary storage capacity (internally the SC1 variable) for the uppermost active cell for each row, column location. The new value specified using the storage-alternative parameter is:

$$SC1_{i,j,k} = \Delta r_j \Delta c_i SYTP_{i,j} \quad (1a)$$

$$SYTP_{i,j} = \sum_{l=1}^p Sytp_l m_{i,j} \quad (1b)$$

where

- $SC1_{i,j,k}$ is the primary storage capacity (Anderman and Hill, 2000, p. 9),
- k is the uppermost model layer with an active cell at row i and column j (MODFLOW layers are numbered 1 at the top and the numbers increase with depth, so often k will equal 1 in this situation),
- Δr_j the grid width of column j ,
- Δc_i the grid width of row i ,
- $Sytp_l$ is the value of alternate storage parameter l ,
- p is the number of additive parameters that define the alternate storage factor in cell i,j , and
- $m_{i,j}$ is the multiplication factor for parameter l at row i and column j .

No multiplication by layer thickness occurs, as is required when specific storage is specified. Thus, the set of p storage-alternative parameters defines specific yield. The storage-alternative parameter allows the use of multiplication and zone arrays and additive parameters to define spatial variations of the alternate storage factor.

Support for storage-alternative parameters required modifications to the GWF1HUF2RPGD, GWF1HUF2PARRP, and GWF1HUF2SP subroutines. In addition, a new subroutine GWF1HUF2SYTP is called from the GWF1HUF2SP subroutine.

Sensitivity Process

The Sensitivity Process solves for sensitivity-equation sensitivities, as described by Hill and others (2000, p. 68-69). The equation solved for transient systems is (Hill and others, 2000, p. 68, eq. 22):

$$\begin{aligned} \underline{A}(m) \frac{\partial \underline{h}(m)}{\partial b_\ell} = & - \frac{\partial \underline{A}(m)}{\partial b_\ell} \underline{h}(m) + \frac{\partial \underline{f}(m)}{\partial b_\ell} + \\ & + \frac{\partial \underline{B}(m)}{\partial b_\ell} \underline{h}(m-1) + \underline{B}(m) \frac{\partial \underline{h}(m-1)}{\partial b_\ell}. \end{aligned} \quad m \geq 1 \quad (2)$$

where,

m is the time step,

$$\underline{A}(m) = \frac{-\underline{S}(m)}{\Delta t(m)} + \underline{K} + \underline{P}(m) \quad [L^2/T],$$

$\underline{S}(m)$ is a diagonal matrix of specific storage multiplied by cell volume, or specific yield multiplied by cell area, depending on whether the layer is confined or, if the layer is convertible, the hydraulic head $[L^2]$,

$\Delta t(m)$ is the length of time step m $[T]$,

\underline{K} is a matrix of horizontal and vertical conductances $[L^2/T]$,

$\underline{P}(m)$ is a diagonal matrix of conductances at head-dependent boundaries $[L^2/T]$,

b_ℓ is the ℓ^{th} parameter,

$\underline{h}(m)$ is a vector of hydraulic heads at the end of time step m for all nodes in the finite-difference grid $[L]$,

$\underline{f}(m)$ is a vector containing the $-Q_{i,j,k}$ terms of McDonald and Harbaugh, (1988, p. 2-26, eq. 26) $[L^3/T]$,

$$\underline{B}(m) = \underline{S}(m)/\Delta t(m).$$

The storage-alternative parameters are used to construct elements of matrix $\underline{S}(m)$, and the derivative of these elements with respect to the storage-alternative parameter is needed to solve equation 2. The derivative is calculated by taking the partial derivative of equation 1 with respect to parameter $Sytp_i$ as:

$$\frac{\partial SC1_{i,j,k}}{\partial Sytp_i} = \Delta r_j \Delta c_i m_{i,j} \quad (3)$$

This sensitivity is calculated in the SEN1HUF2FM subroutine.

Simulation Example

The storage-alternative parameter is demonstrated using a synthetic problem derived from test case 2 of Hill and others (2000) that includes features common to a complex three-dimensional ground-water flow model. This complex example also is used to perform regression with observations that exactly equal the correct values and that contain sufficient information to estimate all parameters. This constitutes a test of the sensitivities because the regression can only estimate parameter values correctly if the sensitivities are correct. Test case 2 was similarly used to test sensitivities by Hill and others (2000, p. 160). The test case was modified here by using a single transient stress period of 100 days.

The model grid for the complex example (fig. 2) has uniform cell dimensions of 1,500 meters (m) in both horizontal directions; the thickness of layers 1, 2, and 3 are 500, 750, and 1,500 m, respectively. Constant-head boundaries comprise parts of the western and eastern boundaries, and no flow occurs across the remaining lateral boundaries and the bottom boundary. Springs are represented using either the Drain or General-Head Boundary Packages of McDonald and Harbaugh (1988) and Harbaugh and others (2000). Wells are simulated at selected nodes and have pumpage rates ranging from 100 to 200 m³/d.

The hydraulic-conductivity distribution of the system is divided vertically into three horizons and horizontally into four zones (fig. 2). All four zones are present in the middle horizon; three are present in each of the top and bottom horizons (fig. 2). Each horizon represents a model layer and is defined in the HUF Package using two equal-thickness hydrogeologic units. The hydraulic-conductivity distribution was defined in this manner to test the ability to represent model layers with multiple hydrogeologic units. The hydraulic properties of the model were defined using the 12 parameters listed in table 1.

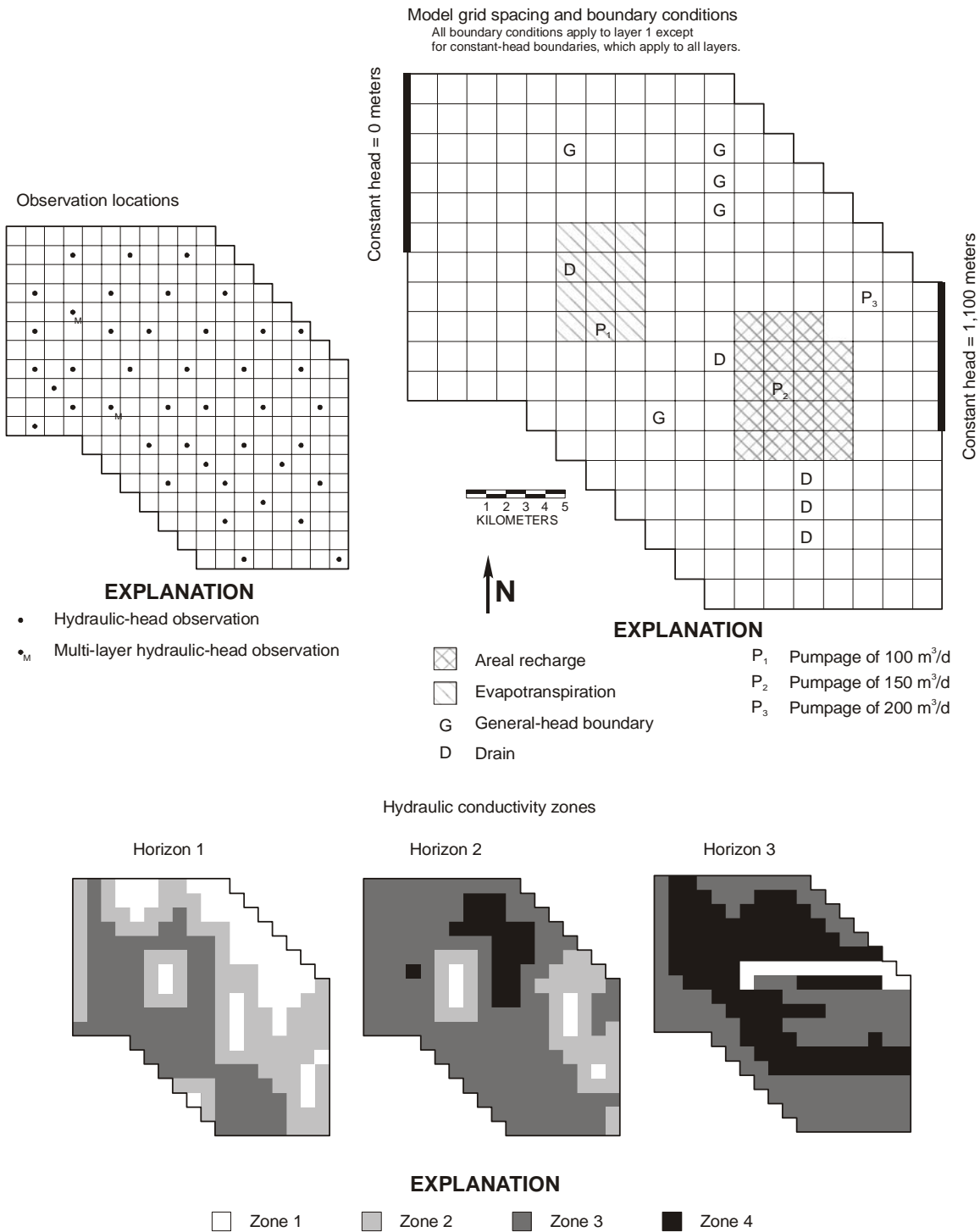


Figure 2. Model grid, boundary conditions, observation locations, and hydraulic-conductivity zones for complex example used to test the calculation of sensitivities. (Modified from Hill and others, 2000.)

The observations (fig. 2) used while estimating parameters consisted of 44 hydraulic heads, 5 drain flows, and 5 general-head boundary flows. The values were generated by running the model with the true parameter values; no random error was added and the observation values equal the simulated values. Composite scaled sensitivities were calculated for the 12 parameters at the initial values listed in table 1 (fig. 3). The sensitivities range in value from 0.22 for the parameter ALTSTOR to 230 for the parameter DRAIN. Using the rule of thumb suggested by Hill (1998, p. 38), the fact that these values span a range of more than two orders of magnitude indicates that estimating all the parameter values by regression may be problematic. The range is just slightly larger than three orders of magnitude. An attempt to estimate all 12 parameters using regression was accomplished successfully using the initial values in table 1. The success of the regression constitutes a test of the sensitivities calculated for the storage-alternative parameter type and indicates that they are calculated correctly.

Table 1. Labels, descriptions, and true and initial values for the parameters for the complex example illustrating the SYTP parameter
[m/d, meters per day; m²/d, square meters per day; --, no units]

Label	Description	Units	True Value	Initial Value
HK1	Horizontal hydraulic conductivity of zone 1	m/d	1.00	1.3
HK2	Horizontal hydraulic conductivity of zone 2	m/d	1.00x10 ⁻²	1.5x10 ⁻²
HK3	Horizontal hydraulic conductivity of zone 3	m/d	1.00x10 ⁻⁴	1.5x10 ⁻⁴
HK4	Horizontal hydraulic conductivity of zone 4	m/d	1.00x10 ⁻⁶	1.2x10 ⁻⁶
SS	Specific storage for entire model grid	m ⁻¹	1.00x10 ⁻³	1.20x10 ⁻³
ALTSTOR	Alternate storage for entire model grid	--	0.10	0.12
VANI1234	Vertical anisotropy of hydrogeologic units 1 through 4	--	4.0	4.2
VANI56	Vertical anisotropy of hydrogeologic units 5 and 6	--	1.0	1.2
DRAIN	Conductance of the head-dependent boundaries ("D") shown in figure 2 using the Drain Package.	m ² /d	1.00	1.3
GHB	Conductance of head-dependent boundaries ("G") shown in figure 2 represented using the General-Head Boundary Package.	m ² /d	1.00	1.3
RCH	Areal recharge rate applied to the area shown in figure 2	m/d	3.10x10 ⁻⁴	3.3x10 ⁻⁴
ETM	Maximum evapotranspiration rate applied to the area shown in figure 2	m/d	4.00x10 ⁻⁴	4.20x10 ⁻⁴

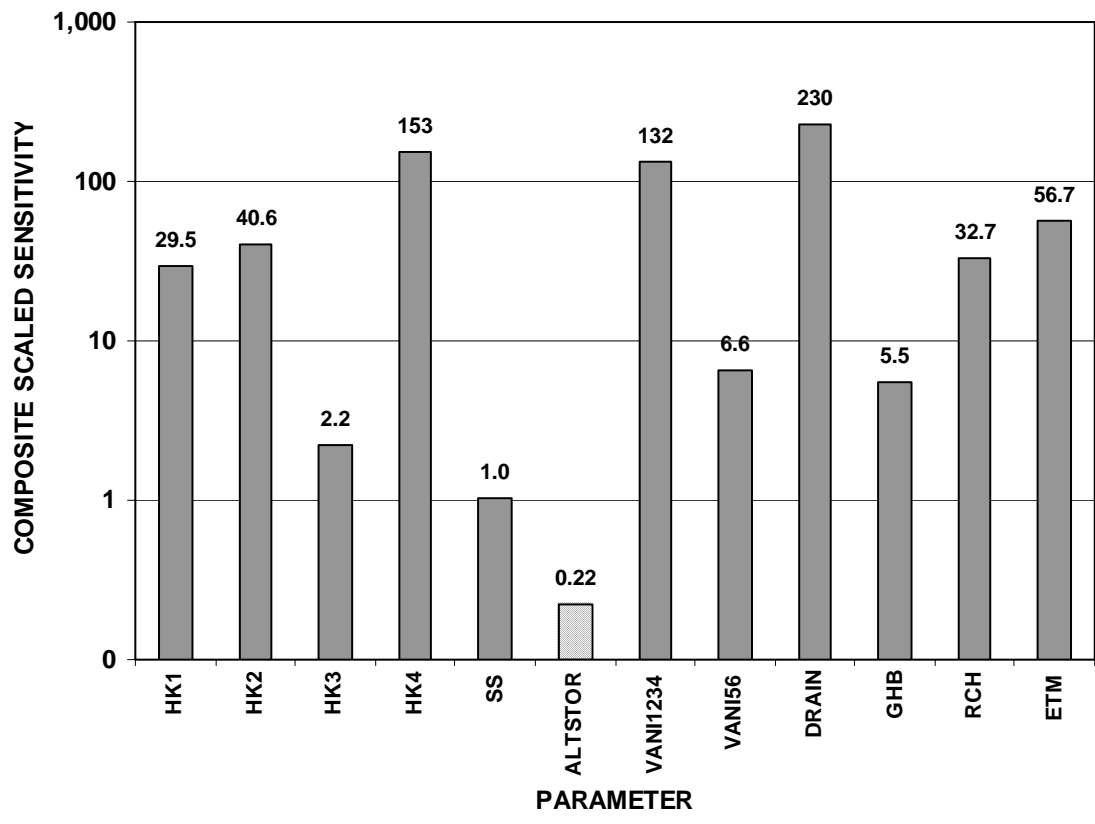


Figure 3. Composite scaled sensitivities at the true values for parameters listed in table 1. Sensitivity for parameter ALTSTOR shown with cross hatching.

FLOWS IN HYDROGEOLOGIC UNITS

The HUF Package was modified to compute flows that occur through hydrogeologic units using MODFLOW-calculated flows through model layers. This means water budgets for hydrogeologic units can be calculated. In addition, the hydrogeologic-unit definition can be used to improve the calculation of transport through the model grid.

Modified Input Instructions

Cell-face flows within hydrogeologic units are calculated when a new variable, IOHUFFLOWS is greater than zero. The new variable has been added to the end of the first item of the HUF Package input file,. The modified input instructions for the HUF Package are shown in Appendix A.

Using the Output

The output from this capability is compatible with existing versions of the ZONEBUDGET program (Harbaugh, 1990). The HUF Package only calculates intercell and constant-head flows interpolated to hydrogeologic units; the other packages calculate flows based on model layers. In order to avoid confusion, it is suggested that the HUF interpolated flows be written to one binary output file and flows for the other package files be written to one or more separate binary files.

Calculation of Flows in Hydrogeologic Units

Horizontal cell-face flows within a hydrogeologic unit are calculated by adding contributions from the model layers that contain the hydrogeologic unit. For each model layer, the flow is calculated using the horizontal conductance attributable to the hydrogeologic unit, and the head gradient within the model layer. These are obtained as described in the following sections. A basic principle is that the flows calculated for the hydrogeologic unit within a model layer need to sum to the flow calculated by MODFLOW for the model layer. This ensures that the hydrogeologic-unit water budget balances the finite-difference cell water-budget computed by MODFLOW.

Conductances

The conductances attributable to the hydrogeologic units within a model layer are additive. That is, they add to the conductance used for the model layer.

The equivalent conductance for the material of hydrogeologic unit g between cell centers in column j and $j+1$ in figure 4 is calculated as:

$$CR_{g,i,j+1/2,k} = 2\Delta c_i \frac{TR_{g,i,j,k} TR_{g,i,j+1,k}}{TR_{g,i,j,k} \Delta r_{j+1} + TR_{g,i,j+1,k} \Delta r_j} \quad (4)$$

where

$TR_{g,i,j,k}$ is the transmissivity of the unit within the cell [L^2/T], calculated as

$$TR_{g,i,j,k} = KH_{i,j,g} thk_{g,i,j,k},$$

$KH_{i,j,g}$ is the horizontal hydraulic conductivity of the unit [L/T],

$thk_{g,i,j,k}$ is the saturated thickness of the unit within the cell [L],

Δc_i is the cell width of row i [L], and

Δr_j is the cell width of column j [L].

This situation is shown on the left side in figure 4, where the j subscripts in equation 4 would be incremented one column to the left.

If a unit g pinches out so that it is only present in one of the cells, the conductance is calculated using a thickness equivalent to the thickness of unit g in the adjacent cell. This situation is shown on the right side of figure 4.

Head Gradient

The HUF Package can interpolate hydraulic heads to hydrogeologic units (Anderman and Hill, 2000, p. 10). However, these heads cannot be used to calculate flows in hydrogeologic units. This is because the interpolated heads produce composite layer flows that in general do not match the model-layer flows calculated by MODFLOW. Table 2 and the model cells shown in figure 5 are used to illustrate the problem. Table 2a shows that the heads vertically interpolated to the hydrogeologic units produce flows that sum over model layers to values that differ from the flows simulated by MODFLOW in the model layers. The result is that the cell water budget is not balanced using hydrogeologic-unit flows calculated with interpolated head gradients.

HUF Imposes Model Grid

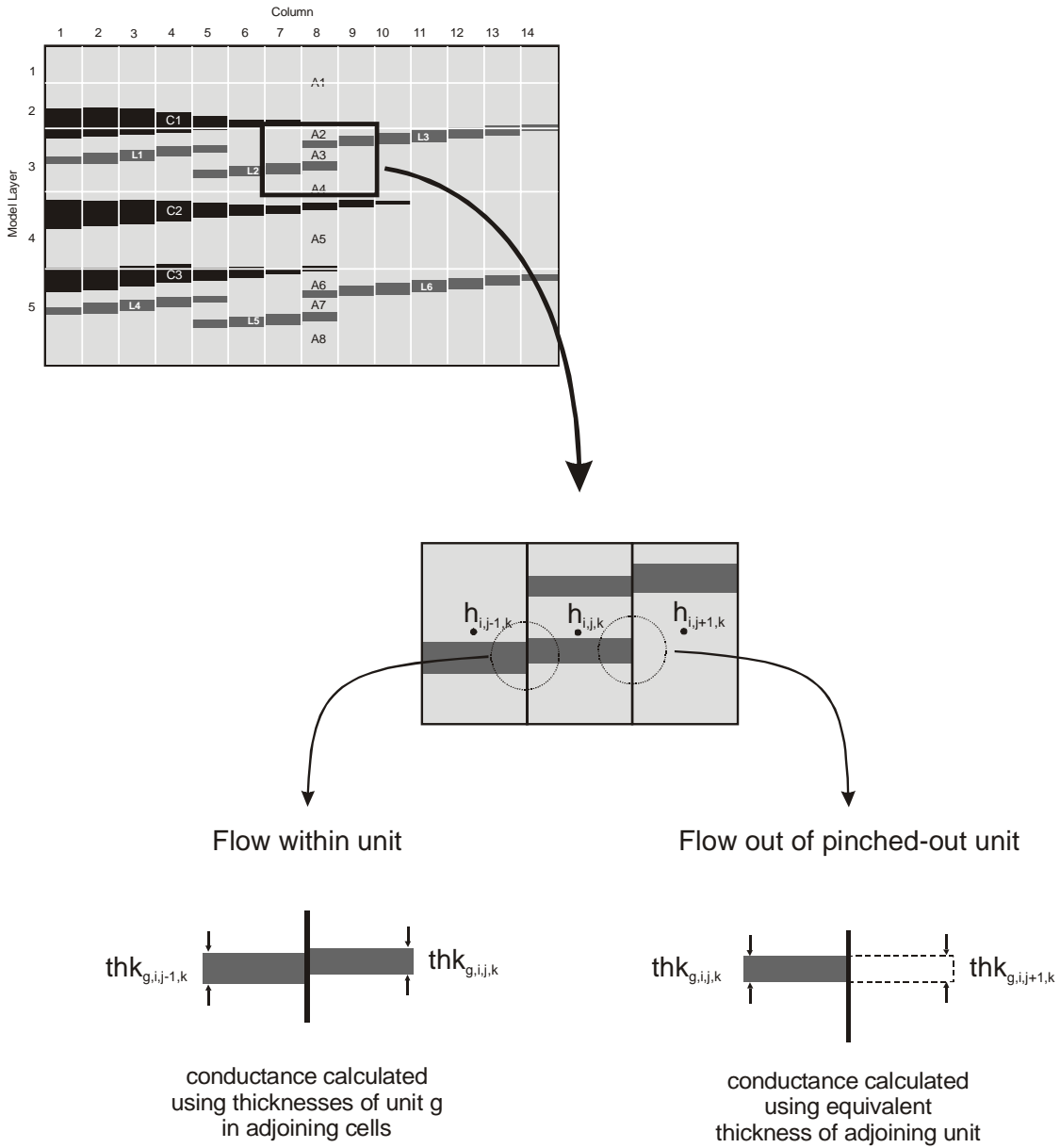


Figure 4. Calculation of equivalent conductance and cell-face flows in a hydrogeologic unit.

To calculate flows for the hydrogeologic units that are consistent with the flows calculated for model layers by MODFLOW, it is necessary to use the heads calculated for each model layer at all vertical positions in the model layer. When these heads are used with conductances calculated for the given hydrogeologic unit, the flow budgets will balance. This method works because the hydrogeologic-unit conductances calculated as described above always sum to the model layer conductances. Thus, if the flows for all units within a given layer are

calculated using the same head gradient used in the model-layer calculation, the resulting flows will sum to the flow calculated by MODFLOW within the model layer.

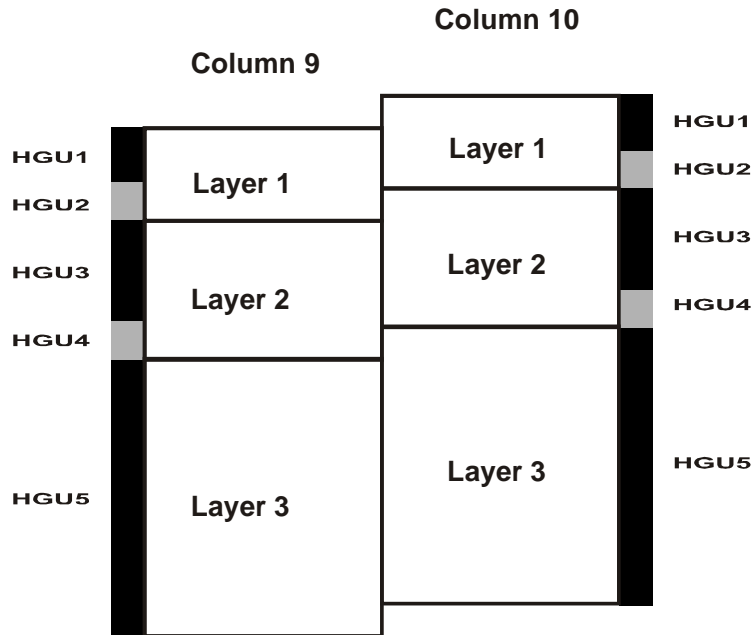


Figure 5. Finite-difference grid cells representing model layers and the hydrogeologic-unit (HGU) definition that applies to each of the cells.

Table 2. Discrepancies between flows accumulated from hydrogeologic units within model layers and MODFLOW-calculated model-layer flows using hydrogeologic-unit heads interpolated vertically and using model-layer heads at all elevations within a model layer. [Unit, hydrogeologic unit; TR9, TR10, transmissivity for the hydrogeologic unit in column 9 or 10 of figure 3, respectively; CR, conductance along rows calculated for hydrogeologic units as in equation 4 and calculated for model layers as in Anderman and Hill (2000, p. 8); H9, H10, hydraulic head used for the midpoint of the hydrogeologic unit or model layer; dH, H9 minus H10 for the hydrogeologic unit or model layer; Error, error in flow calculated for the model layer relative to the flow calculated by MODFLOW; K, hydraulic conductivity; T, transmissivity]

(a) Flow in model layers

Layer	TR9	TR10	CR (m ² /d)	H9 (m)	H10 (m)	dH (m)	Flow (m ³ /d)
1	4.97E-02	4.95E-02	4.96E-02	1126.56	1307.71	-181.15	-8.99
2	7.50E-02	7.50E-02	7.50E-02	1133.48	1275.29	-141.81	-10.64
3	1.50E-03	1.50E-01	2.97E-03	1177.63	1320.29	-142.66	-0.42

(b) Flow in hydrogeologic units using heads interpolated vertically to the centers of the hydrogeologic units.

Unit	TR9	TR10	CR (m ² /d)	H9 (m)	H10 (m)	dH (m)	Flow (m ³ /d)	Flow in Layer	Error
HGU1	2.97E-02	2.95E-02	2.96E-02	1125.47	1312.78	-187.31	-5.55	-8.98	-0.1%
HGU2	2.00E-02	2.00E-02	2.00E-02	1128.22	1299.93	-171.71	-3.43		
HGU3	5.50E-02	5.50E-02	5.50E-02	1132.38	1280.48	-148.10	-8.15	-11.41	7.3%
HGU4	2.00E-02	2.00E-02	2.00E-02	1134.12	1297.29	-163.17	-3.26		
HGU5	1.50E-03	1.50E-01	2.97E-03	1177.63	1320.29	-142.66	-0.42	-0.42	0.0%

(c) Flow in hydrogeologic units using model-layer heads.

Unit	TR9	TR10	CR (m ² /d)	H9 (m)	H10 (m)	dH (m)	Flow (m ³ /d)	Flow in Layer	Error
HGU1	2.97E-02	2.95E-02	2.96E-02	1126.56	1307.71	-181.15	-5.37	-8.99	0.0%
HGU2	2.00E-02	2.00E-02	2.00E-02	1126.56	1307.71	-181.15	-3.62		
HGU3	5.50E-02	5.50E-02	5.50E-02	1133.48	1275.29	-141.81	-7.80	-10.64	0.0%
HGU4	2.00E-02	2.00E-02	2.00E-02	1133.48	1275.29	-141.81	-2.84		
HGU5	1.50E-03	1.50E-01	2.97E-03	1177.63	1320.29	-142.66	-0.42	-0.42	0.0%

(d) Hydrogeologic-unit thickness, hydraulic conductivity, and transmissivity

Unit	Column 9				Column 10			
	Thickness(m)	K (m/d)	T (m ² /d)	Total T	Thickness	K (m/d)	T (m ² /d)	Layer T
HGU1	297.00	1.00E-04	2.97E-02	4.97E-02	295.44	1.00E-04	2.95E-02	4.95E-02
HGU2	200.00	1.00E-04	2.00E-02		200.00	1.00E-04	2.00E-02	
HGU3	550.00	1.00E-04	5.50E-02	7.50E-02	550.00	1.00E-04	5.50E-02	7.50E-02
HGU4	200.00	1.00E-04	2.00E-02		200.00	1.00E-04	2.00E-02	
HGU5	1500.00	1.00E-06	1.50E-03	1.50E-03	1500.00	1.00E-04	1.50E-01	1.50E-01

Program Changes to the Ground-Water Flow Process

Modifications to the Ground-Water Flow Process of MODFLOW-2000 were necessary to print flows for hydrogeologic units. Specifically, subroutine GWF1HUF2OT was modified to calculate and print flows for hydrogeologic units by calling a new subroutine, SGWF1HUF2FLOT.

THE HYDRAULIC-CONDUCTIVITY DEPTH-DEPENDENCE (KDEP) CAPABILITY

Hydraulic conductivity can decline systematically with depth (Taylor and others, 2001; Whittemore and others, 1993). While the best function to use is not always clear, exponential decay is commonly assumed, and is used in this report.

The capability of the HUF Package presented here allows a depth-dependence parameter type, KDEP, that controls the exponential decay of horizontal hydraulic conductivity of hydrogeologic units with depth. This capability allows sensitivities to be calculated and optimal parameter values to be estimated. The use of a depth-dependence parameter also affects the vertical hydraulic conductance when VANI parameters are used. The reference surface from which depth is measured can be defined as the TOP array in the discretization input file (Harbaugh and others, 2000, p. 45) or as a separate array defined in an input file with other depth-dependence parameter related input.

This section defines the exponential depth-dependence function used to modify hydraulic conductivity with depth and discusses depth-dependence parameters and sensitivities calculated for the depth-dependence parameters. Except for the definition of depth decay, the discussion here is conceptual; the relevant equations are presented in Appendix B.

Definition of Exponential Depth Dependence

With exponential decay, hydraulic conductivity decreases with depth using the following function:

$$K_{Depth} = K_{Surface} 10^{-\lambda d} \quad (5)$$

where

- K_{Depth} is the hydraulic conductivity at depth d [L/T],
- $K_{Surface}$ is the hydraulic conductivity projected to a reference surface [L/T]
- λ is the depth-dependence coefficient, which can be defined using parameters [L⁻¹], and
- d is the depth below the reference surface [L].

The decline in hydraulic conductivity with depth relative to the reference-surface hydraulic conductivity is shown for several values of the depth-dependence coefficient λ in figure 6. For

larger values of the depth-dependence coefficient, the hydraulic conductivity initially decreases more rapidly with depth than for smaller values.

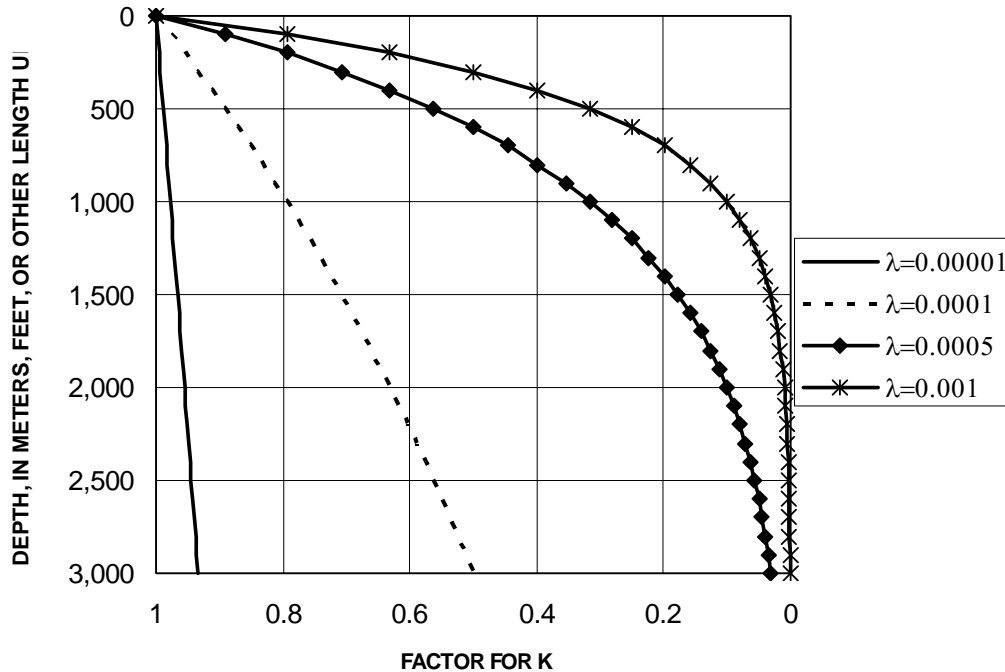


Figure 6. Decline with depth of hydraulic conductivity relative to the reference-surface hydraulic conductivity for several depth-dependence coefficient values. Units, such as per meter or per foot, are not listed for the depth-dependence coefficient because the only requirement is that the unit be the inverse of the unit of depth.

Depth-Dependence Parameters

Determining the value of the depth-dependence coefficient directly from hydraulic-conductivity data can be difficult because in most situations such data are scarce, depth decay is obscured by variability caused by other factors, and measurement error is substantial. Often measured hydraulic heads, flows, and concentrations provide the most definitive information concerning depth decay. Using these measurements to determine the depth-dependence coefficient requires that the coefficient be defined using parameters in MODFLOW-2000.

Zone and multiplication arrays (Harbaugh and others, 2000, p. 14-16) can be used in conjunction with the depth-dependence parameters to define spatial variation of the depth-dependence coefficients. Using zone arrays, the depth-dependence coefficient can, for example, be defined to equal different parameters in different hydrogeologic units or different regions of

one or more hydrogeologic units. Using multiplication arrays, expected spatial variations in the depth-dependence coefficient can be represented. For example, changes in compressibility indicated by geologic data can be used to indicate spatial variations in the depth-dependence coefficient, and this information can be used to define a multiplication array.

Like most parameters in MODFLOW-2000, depth-dependence parameters are additive, as described by Harbaugh and others (2000, p. 16-19). Thus, parameters can be used to represent the depth-dependence coefficient with interpolation methods such as kriging. Kriging can be accomplished by defining a parameter at each of the kriging points and assigning to each parameter a multiplication array. The multiplication array would be obtained by kriging the points of interest with a value of 1.0 assigned to the location associated with this parameter, and a value of 0.0 assigned to all other kriging points.

An issue of concern is that the uncertainty in the specification of the zone and multiplication arrays and of any interpolation scheme used is not fully reflected in uncertainty measures based only on the parameter variance-covariance matrix. This is discussed by Hill (1998).

Modified Input Instructions

The depth-dependence parameter capability requires that the keyword 'KDEP' be specified in the MODFLOW-2000 Name file (Harbaugh and others, 2000, p. 7) and that a new input file be constructed. The new input is described in Appendix B.

Program Changes

The program changes required for the hydraulic-conductivity depth-dependence capability are presented in Appendix B.

Simulation Example

The depth-dependence parameter is demonstrated using the synthetic problem presented previously in this report for the storage-alternative parameter. A single depth-dependence type parameter was defined that applied the depth-dependence coefficient to all hydrogeologic units of the entire model grid. Composite scaled sensitivities (fig. 7) were calculated for the 10 parameters at the true values listed in table 3. The sensitivities range in value from 0.04 for the HK4 parameter to 87.1 for the RCH parameter. An attempt to estimate all 10 parameters using

regression was accomplished successfully using the initial values in table 3. The success of the regression constitutes a test of the sensitivities calculated for the depth-dependence type parameter and indicates that they are calculated correctly.

Table 3. Labels, descriptions, and true and initial values for the parameters for the complex example illustrating the use of a depth-dependence type parameter [m/d, meters per day; m²/d, square meters per day; --, no units]

Label	Description	Units	True Value	Initial Value
HK1	Horizontal hydraulic conductivity of zone 1	m/d	1.00	1.3
HK2	Horizontal hydraulic conductivity of zone 2	m/d	1.00x10 ⁻²	1.5x10 ⁻²
HK3	Horizontal hydraulic conductivity of zone 3	m/d	1.00x10 ⁻⁴	1.5x10 ⁻⁴
HK4	Horizontal hydraulic conductivity of zone 4	m/d	1.00x10 ⁻⁶	1.2x10 ⁻⁶
DEPCOFF	Depth-dependence coefficient for entire model grid	m ⁻¹	1.00x10 ⁻³	3.00x10 ⁻³
VANI1234	Vertical anisotropy of hydrogeologic units 1 through 4	--	4.0	4.2
VANI56	Vertical anisotropy of hydrogeologic units 5 and 6	--	1.0	1.2
DRAIN	Conductance of the head-dependent boundaries (“D”) shown in figure 2 using the Drain Package.	m ² /d	1.00	1.3
GHB	Conductance of head-dependent boundaries (“G”) shown in figure 2 represented using the General-Head Boundary Package.	m ² /d	1.00	1.3
RCH	Areal recharge rate applied to the area shown in figure 2	m/d	3.10x10 ⁻⁴	3.3x10 ⁻⁴

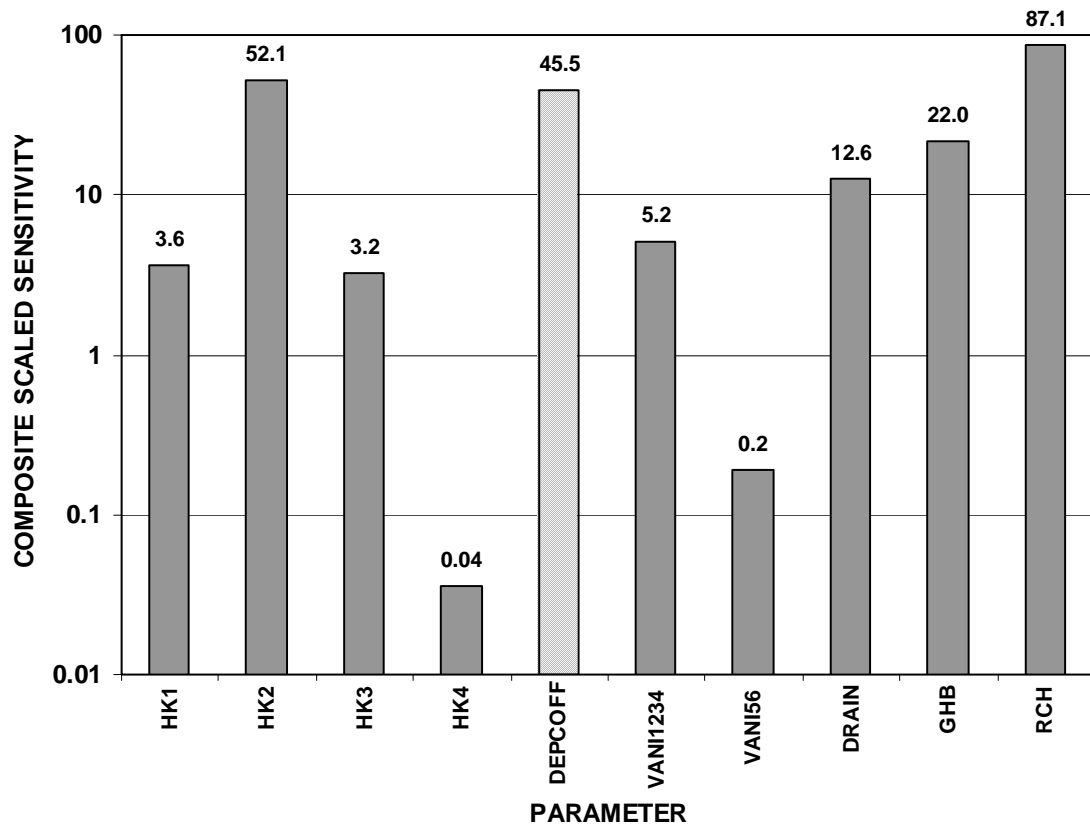


Figure 7. Composite scaled sensitivities at the true values for parameters listed in table 2. Sensitivity for the DEPCOFF parameter is shown with cross hatching.

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APPENDIX A: MODIFIED INPUT FILE FOR THE HYDROGEOLOGIC-UNIT FLOW (HUF) PACKAGE

Input for the modified HUF Package is read from the file that has type "HUF2" in the name file. Free format is used for reading all values. Changes included that are new to version 2 are underlined and include the new variable IOUHUFFLOWS in item 1 and the new parameter type SYTP listed in the definition of the variable PARTYP of item 10. Optional variables are shown in brackets.

Input File

FOR EACH SIMULATION

0. [#Text]
Item 0 is optional -- “#” must be in column 1. Item 0 can be repeated multiple times.
1. IHUF^{CB} HD^{RY} NHUF^F NPHUF^F IOHUFHEADS IOUHUFFLOWS
2. LTHUF (NLAY)
3. LAYWT (NLAY)
4. [WETFCT IWETIT IHDWET]
(Include Item 4 only if LAYWT indicates at least one wettable layer.)
5. [WETDRY (NCOL, NROW)]
Repeat Item 5 for each layer for which LAYWET is not 0.
Arrays are read by the array-reading utility module, U2DREL.
6. HGUNAM
7. TOP (NCOL, NROW)
8. THCK (NCOL, NROW)
Repeat Items 6-8 for each hydrogeologic unit to be defined (that is, NHUF times).
9. HGUNAM HGUHANI HGUUVANI
Repeat Item 9 for each hydrogeologic unit. If HGUNAM is set to “ALL”, HGUHANI and HGUUVANI define values for all hydrogeologic units, and only one Item 9 is necessary. Otherwise, HGUNAM must correspond to one of the names defined in Item 6, and there must be NHUF repetitions of Item 9. The repetitions can be in any order.
10. PARNAM PARTYP Parval NCLU
11. HGUNAM Mltarr Zonarr IZ
Each Item 11 record is called a parameter cluster. Repeat Item 11 NCLU times. Repeat Items 10-11 for each parameter to be defined (that is, NPHUF times).
12. [**PRINT** HGUNAM PRINTCODE PRINTFLAGS]
Item 12 is optional and is included only for hydrogeologic units for which printing is desired. Item 12 must start with the word PRINT. If HGUNAM is set to ALL, PRINTCODE and PRINTFLAGS are set for all hydrogeologic units, and only one Item 12 is necessary. Otherwise, HGUNAM must correspond to one of the names defined in Item 6.

Explanation of Variables Read by the Hydrogeologic-Unit Flow Package

Text – is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The “#” character must be in column 1. Text is printed when the file is read.

IHUFEB – is a flag and a unit number.

> 0 – the unit number to which cell-by-cell flow terms will be written when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control (Harbaugh and others, 2000, p. 55). The terms that are saved are storage, constant-head flow, and flow between adjacent cells.

0 – cell-by-cell flow terms will not be written.

< 0 – cell-by-cell flow for constant-head cells will be written in the listing file when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control. Cell-by-cell flow to storage and between adjacent cells will not be written to any file.

HDRY – is the head that is assigned to cells that are converted to dry during a simulation.

Although this value plays no role in the model calculations, it is useful as an indicator when looking at the resulting heads that are output from the model. HDRY is thus similar to HNOFLO in the Basic Package, which is the value assigned to cells that are no-flow cells at the start of a model simulation.

NHUF – is the number of hydrogeologic units defined using the HUF package.

NPHUF – is the number of HUF parameters.

IOHUFHEADS – is a flag and a unit number.

0 – interpolated heads will not be written.

> 0 – calculated heads will be interpolated and written on unit IOHUFHEADS for each hydrogeologic unit using the format defined in the output-control file.

IOHUFFLOWS – is a flag and a unit number.

0 – interpolated flows will not be written.

> 0 – calculated cell-by-cell flows will be interpolated and written on unit IOHUFFLOWS for each hydrogeologic unit using the format defined in the output-control file.

LTHUF – is a flag specifying the layer type. Read one value for each layer; each element holds the code for the respective layer. There is a limit of 200 layers. Use as many records as needed to enter a value for each layer.

0 – indicates a confined layer.
not 0 – indicates a convertible layer.

LAYWT – is a flag that indicates if wetting is active. Read one value per layer.

0 – indicates wetting is inactive.
1 – indicates wetting is active.

WETFCT – is a factor that is included in the calculation of the head that is initially established at a cell when the cell is converted from dry to wet. (See IHDWET.)

IWETIT – is the iteration interval for attempting to wet cells. Wetting is attempted every IWETIT iterations. If using the preconditioned conjugate gradient (PCG) solver (Hill, 1990), this applies to outer iterations, not inner iterations. If IWETIT is 0, it is changed to 1.

IHDWET – is a flag that determines which equation is used to define the initial head at cells that become wet:

If IHDWET = 0, equation 3a from McDonald and others (1992) is used:

$$h = BOT + WETFCT (h_n - BOT)$$

If IHDWET is not 0, equation 3b from McDonald and others (1992) is used:

$$h = BOT + WETFCT (WETDRY)$$

WETDRY – is a combination of the wetting threshold and a flag to indicate which neighboring cells can cause a cell to become wet. If WETDRY < 0, only the cell below a dry cell can cause the cell to become wet. If WETDRY > 0, the cell below a dry cell and the four horizontally adjacent cells can cause a cell to become wet. If WETDRY is 0, the cell cannot be wetted. The absolute value of WETDRY is the wetting threshold. When the sum of BOT and the absolute value of WETDRY at a dry cell is equaled or exceeded by the head at an adjacent cell, the cell is wetted. Read only if LAYTYP is not 0 and LAYWET is not 0.

HGUNAM – is the name of the hydrogeologic unit. This name can consist of up to 10 characters and is not case sensitive.

TOP – is the elevation of the top of the hydrogeologic unit.

THCK – is the thickness of the hydrogeologic unit.

HGUHANI – is a flag and a horizontal anisotropy value for a hydrogeologic unit. Horizontal anisotropy is the ratio of hydraulic conductivity along columns to hydraulic conductivity along rows. Read one value for each hydrogeologic unit unless HGUNAM is set to ALL.

0 – indicates that horizontal anisotropy will be defined using a HANI parameter.

> 0 – HGUHANI is the horizontal anisotropy of the entire hydrogeologic unit. Value is ignored if a HANI parameter is defined for the corresponding hydrogeologic unit.

HGUVANI – is a flag that indicates whether array VK is vertical hydraulic conductivity or the ratio of horizontal to vertical hydraulic conductivity. Read only one value for each hydrogeologic unit unless HGUNAM is set to ALL.

0 – indicates VK is vertical hydraulic conductivity (VK parameter must be used).

> 0 – indicates VK is the ratio of horizontal to vertical hydraulic conductivity and HGUVANI is the vertical anisotropy of the entire hydrogeologic unit. Value is ignored if a VANI parameter is defined for the corresponding hydrogeologic unit.

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 HUF Package, the allowed parameter types are:

HK – defines variable HK, horizontal hydraulic conductivity.

HANI – defines variable HANI, horizontal anisotropy.

VK – defines variable VK, vertical hydraulic conductivity, for units for which HGUVANI is set to zero.

VANI – defines variable VANI, vertical anisotropy, for units for which HGUVANI is set greater than zero.

SS – defines variable Ss, the specific storage.

SY – defines variable Sy, the specific yield.

SYTP – when all model layers are confined, defines the storage coefficient for the top active cell at each row, column location. The value specified is not multiplied by model layer thickness. When SYTP is specified as the parameter type, HGUNAM of item 11 needs to be set to SYTP.

Parval – is the initial value of the parameter; however, this value can be replaced by a value specified in the Sensitivity Process input file.

NCLU – is the number of clusters required to define the parameter. Each Item-11 record is a cluster (variables HGUNAM, Mltarr, Zonarr, and IZ).

HGUNAM – is the hydrogeologic unit to which the parameter applies. When PARTYP = SYTP, HGUNAM must be set to SYTP.

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 hydrogeologic unit 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. The first zero or non-numeric value terminates the list. These values are not used if Zonarr is specified as “ALL”.

PRINTCODE – determines the format for printing the values of the hydraulic-property arrays for the hydrogeologic unit as defined by parameters. The print codes are the same as those used in an array control record (Harbaugh and others, 2000, p. 87).

PRINTFLAGS – determines the hydraulic-property arrays to be printed and must be set to “ALL” or any of the following: “HK”, “HANI”, “VK”, “SS”, or “SY”. Arrays will be printed only for those properties that are listed. When VK is specified, the property printed depends on the setting of HGUVANI.

APPENDIX B: INPUT INSTRUCTIONS, OUTPUT, AND PROGRAM DESCRIPTION OF THE HYDRAULIC-CONDUCTIVITY DEPTH-DEPENDENCE (KDEP) CAPABILITY

The depth-dependence capability is a modification to the existing HUF Package (Anderman and Hill, 2000). This section describes the new input file needed with the depth-dependence capability and the changes in the HUF Package output files resulting from using the depth-dependence capability. There are no changes in the HUF Package output files if the depth-dependence capability is not used.

Depth-Dependence Capability Input Instructions

Input for the Hydraulic-Conductivity Depth-Dependence capability is read from the file that has type “KDEP” in the Name file. Free format is used for reading all values.

FOR EACH SIMULATION

0. [#Text]
Item 0 is optional -- “#” must be in column 1. Item 0 can be repeated multiple times.
1. NPKDEP IFKDEP
2. RS (NCOL, NROW)
Include Item 2 only if IFKDEP is greater than 0. Item 2 is read using the array-reading utility module U2DREL (Harbaugh and others, 2000, p. 86-88).
3. PARNAM PARTYP Parval NCLU
4. HGUNAM Mltarr Zonarr IZ
Each Item 4 record is called a parameter cluster. Repeat Item 4 NCLU times.
Repeat Items 3 and 4 for each parameter to be defined (that is, NPKDEP times).

Explanation of Variables Read by the Depth-Dependence Capability

Text – is a character variable (up to 199 characters) that starts in column 2. Any characters can be included in Text. The “#” character must be in column 1. Text is printed when the file is read.

NPKDEP – is the number of depth-dependence parameters.

IFKDEP – is a flag indicating the source of the array specifying reference-surface elevation.

0 – the TOP array specified in the Discretization Package Input File will be used.

> 0 – an array will be specified in Item 2.

RS – is the elevation of the reference surface to be used to calculate the depth.

PARNAM – is the name of a depth-dependence 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 depth-dependence capability, the only allowed parameter type is:

KDEP – defines the depth-dependence coefficient used to modify horizontal hydraulic conductivity with depth for the hydrogeologic unit(s) specified in Item 4. NOTE: horizontal hydraulic conductivity is only modified for cells in units defined by depth-dependence parameters and not for other cells, so depth-dependence parameters do not need to be specified for the entire model.

Parval – is the initial value of the parameter; however, this value can be replaced by a value specified 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 Item-4 record is a cluster (variables HGUNAM, Mltarr, Zonarr, and IZ).

HGUNAM – is the hydrogeologic unit to which the parameter applies.

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 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. The first zero or non-numeric value terminates the list. These values are not used if Zonarr is specified as “ALL”.

Example Depth-Dependence Capability Input File

The following lines of data illustrate the definition of the depth-dependence type parameter for the three-dimensional simulation presented in the text. In this definition, the parameter value of 0.001 is applied to all zones in each hydrogeologic unit.

```
#KDEP Parameter for HUF Test Case 2, Variant 7
1 1
INTERNAL      1.0 (7f10.2)
0.00 466.66 970.89 979.17 979.48 980.07 1025.00
1123.69 1184.28 1185.76 1186.51 9999.00 9999.00 9999.00
9999.00 9999.00 9999.00 9999.00 9999.00 9999.00 9999.00
0.00 460.53 968.83 979.02 979.21 979.77 1015.11
1103.04 1170.61 1186.49 1187.26 1188.65 9999.00 9999.00
9999.00 9999.00 9999.00 9999.00 9999.00 9999.00 9999.00
0.00 432.95 961.24 973.60 978.55 957.74 987.47
1088.84 1179.69 1186.78 1187.39 1190.05 1191.79 9999.00
9999.00 9999.00 9999.00 9999.00 9999.00 9999.00 9999.00
0.00 291.69 752.49 967.22 971.47 964.35 990.43
1082.56 1176.54 1177.24 1159.66 1192.36 1193.54 1194.92
9999.00 9999.00 9999.00 9999.00 9999.00 9999.00 9999.00
0.00 220.86 552.04 799.15 897.53 929.42 956.07
983.73 1077.55 1147.71 1154.33 1194.15 1195.09 1196.29
1197.29 9999.00 9999.00 9999.00 9999.00 9999.00 9999.00
0.00 188.80 463.00 692.59 852.09 892.57 932.76
906.94 1007.63 1147.73 1201.15 1195.77 1196.37 1197.88
1198.28 1198.34 9999.00 9999.00 9999.00 9999.00 9999.00
27.65 189.71 420.51 653.17 857.06 922.11 1014.73
951.16 1023.76 1183.96 1259.68 1242.39 1215.40 1200.60
1200.03 1198.83 1197.33 9999.00 9999.00 9999.00 9999.00
50.33 209.99 431.34 642.47 850.77 944.38 1014.46
953.31 1036.80 1233.05 1337.05 1346.38 1256.78 1205.05
1203.72 1200.92 1197.30 1100.00 1100.00 1100.00 1100.00
67.18 233.93 444.97 634.74 835.28 925.80 971.05
931.50 1049.61 1275.58 1407.16 1449.87 1356.59 1209.95
1209.11 1204.70 1176.94 1100.00 1100.00 1100.00 1100.00
77.44 262.59 462.38 635.42 812.44 951.31 990.28
999.73 1107.81 1286.30 1395.35 1453.25 1424.78 1276.80
1214.27 1202.18 1159.09 1100.00 1100.00 1100.00 1100.00
207.65 336.39 484.48 640.95 809.63 926.59 996.19
1045.80 1129.56 1312.27 1441.08 1456.96 1447.99 1315.52
1217.30 1204.81 1157.15 1100.00 1100.00 1100.00 1100.00
9999.00 9999.00 9999.00 9999.00 871.62 949.88 1018.16
1062.88 1036.73 1312.10 1459.70 1459.79 1479.20 1375.99
1284.80 1218.50 1164.71 1100.00 1100.00 1100.00 1100.00
9999.00 9999.00 9999.00 9999.00 9999.00 1000.38 1063.05
1123.83 1184.97 1336.58 1482.97 1513.53 1515.39 1419.18
1314.91 1228.81 1181.96 1153.66 1153.66 1153.66 1153.66
9999.00 9999.00 9999.00 9999.00 9999.00 9999.00 1117.51
1183.17 1225.02 1283.48 1375.39 1404.99 1388.08 1333.35
1276.05 1215.86 1193.01 1177.67 1177.67 1177.67 1177.67
9999.00 9999.00 9999.00 9999.00 9999.00 9999.00 9999.00
1239.21 1241.07 1242.52 1282.86 1303.60 1286.91 1219.00
1240.73 1206.68 1193.28 1188.76 1188.76 1188.76 1188.76
9999.00 9999.00 9999.00 9999.00 9999.00 9999.00 9999.00
9999.00 1241.55 1242.06 1255.55 1262.52 1249.10 1206.20
1216.15 1197.47 1193.35 1192.28 1192.28 1192.28 1192.28
9999.00 9999.00 9999.00 9999.00 9999.00 9999.00 9999.00
9999.00 9999.00 1242.22 1246.68 1247.25 1238.52 1221.48
1209.43 1195.85 1194.18 1193.66 1193.66 1193.66 1193.66
9999.00 9999.00 9999.00 9999.00 9999.00 9999.00 9999.00
9999.00 9999.00 9999.00 1244.51 1242.16 1234.80 1222.75
1208.12 1195.45 1194.60 1194.10 1194.10 1194.10 1194.10
KDEP_ALL KDEP 0.001 6
Item 3: PARNAM PARTYP PARVAL NCLU
Item 4: HGU MLTARR ZONARR IZ
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Depth-Dependence Capability Output

There is no special output for the depth-dependence capability.

Program Changes for the Depth-Dependence Capability

Support for the depth-dependence capability is implemented in both the Ground-Water Flow Process and the Sensitivity Process of MODFLOW-2000. The changes made to each of the processes is shown in the following sections.

Contribution to the MODFLOW Ground-Water Flow Process

The decay of hydraulic conductivity with depth is assumed to vary according to equation 5. In the original HUF Package, transmissivity in the row direction $TR_{i,j,k}$ for a cell at row i , column j , and layer k is calculated as (Anderman and Hill, 2000, p. 8):

$$TR_{i,j,k} = \sum_{g=1}^n KH_{i,j,g} thk_{g,i,j,k} , \quad (B-1)$$

where

- n is the number of hydrogeologic units within the finite-difference cell;
- $KH_{i,j,g}$ is equal to $\sum_{l=1}^p Kh_l m_{l,i,j,g}$;
- Kh_l is the value of horizontal hydraulic conductivity parameter l ;
- $thk_{g,i,j,k}$ is the thickness of hydrogeologic unit g in cell i, j, k ;
- p is the number of additive parameters that define the hydraulic conductivity of hydrogeologic unit g ; and
- $m_{l,i,j,g}$ is the multiplication factor for parameter l .

From equation B-1, the transmissivity for a model grid cell accounts for the hydrogeologic units contained in that cell.

The depth-dependence function as a multiplier on the hydraulic conductivity for hydrogeologic units will be defined. In equation B-1, depth decay therefore needs to be applied to the portion of the unit within the cell. A difficulty occurs because the depth-dependence function changes continually with depth, while a single multiplier is needed for equation B-1. The single multiplier is obtained by integrating the function over the interval and dividing it by the interval. Thus,

$$M_{KDEP_{g,i,j,k}} = \frac{\int_{d_1}^{d_2} 10^{-\lambda d} dd}{d_2 - d_1} \quad (B-2)$$

Fundamental calculus shows that

$$\int b^{ax} dx = \frac{1}{a} \frac{b^{ax}}{\ln b} \quad (B-3)$$

so the final hydraulic-conductivity multiplier is

$$M_{KDEP_{g,i,j,k}} = \frac{10^{-\lambda_{i,j,g} d_{2gi,j,k}} - 10^{-\lambda_{i,j,g} d_{1gi,j,k}}}{-\lambda_{i,j,g} (d_{2gi,j,k} - d_{1gi,j,k}) \ln 10} \quad (B-4)$$

where

- $\lambda_{i,j,g}$ is the depth-dependence coefficient for row i and column j of hydrogeologic unit g ,
- $d_{1gi,j,k}$ is the depth of the top of unit g within the cell at row i and column j of layer k ,
and
- $d_{2gi,j,k}$ is the depth of the bottom of unit g within the cell at row i and column j of layer k .

More generally, like most parameters in MODFLOW-2000 (Harbaugh and others, 2000, p. 16), λ can be multiplied by factors that are unique to each row, column, and hydrogeologic unit, and parameters can be additive. If multipliers are used and the additive option is used, then

$$\lambda_{i,j,g} = \sum_{l=1}^p \lambda_l m_{l,i,j,g} \quad (B-5)$$

where

- λ_l is the value of the depth-dependence coefficient parameter l , and
- $m_{l,i,j,g}$ is the multiplication factor for KDEP parameter l .

The sensitivity equations are developed below with this possibility in mind.

Finally, equation B-1 is then modified to:

$$TR_{i,j,k} = \sum_{g=1}^n M_{KDEP_{g,i,j,k}} KH_{i,j,g} thk_{g,i,j,k} \quad (B-6)$$

Contribution to the MODFLOW Sensitivity Process

To calculate sensitivities for depth-dependence parameters using the sensitivity-equation method requires certain derivatives to be evaluated. For example, the steady-state, confined sensitivity equation is (Anderman and Hill, 2000, p. 78, eq. B-1):

$$\underline{A}(0) \frac{\partial \underline{h}(0)}{\partial b_l} = - \frac{\partial \underline{A}(0)}{\partial b_l} \underline{h}(0) - \frac{\partial \underline{f}(0)}{\partial b_l}, \quad (\text{B-7})$$

where

- $\underline{h}(0)$ is a vector of hydraulic heads [L],
- $\underline{A}(0)$ equals $\underline{K} + \underline{P}(0)$ [L^2/T],
- \underline{K} is a matrix of horizontal and vertical conductances [L^2/T],
- $\underline{P}(0)$ is a diagonal matrix of conductances at head-dependent boundaries [L^2/T],
- $\underline{f}(n)$ is the forcing function [L^3/T], and
- b_l is the l^{th} parameter.

The $\frac{\partial \underline{A}(0)}{\partial b_l}$ terms are non-zero for depth-dependence parameters, and require that derivatives of hydraulic conductances with respect to the depth-dependence parameters be calculated.

Derivative of Horizontal Conductance with respect to a Depth-Dependence Parameter

To calculate the sensitivities of horizontal conductances to a depth-dependence parameter, the derivative of the transmissivity in equation B-6 needs to be calculated with respect to the depth-dependence parameter λ_l :

$$\frac{\partial TR_{i,j,k}}{\partial \lambda_l} = \sum_{g=1}^m \frac{\partial M_{KDEP_{g_{i,j,k}}}}{\partial \lambda_l} KH_{i,j,g} thk_{g_{i,j,k}} \quad (\text{B-8})$$

where

m is the number of intervals of parameter l in cell i,j,k .

In general, the derivative of the depth-dependence function is taken as:

$$\frac{\partial 10^{-\lambda d}}{\partial \lambda_l} = -d 10^{-\lambda d} \ln 10 \quad (\text{B-9})$$

To derive the sensitivity of the hydraulic-conductivity multiplier of equation B-4, the basic calculus relation is used:

$$\frac{\partial}{\partial b} \left[\frac{u}{v} \right] = \frac{v \frac{\partial u}{\partial b} - u \frac{\partial v}{\partial b}}{v^2}. \quad (\text{B-10})$$

where

$$u = 10^{-\lambda_{i,j,g} d_{2gi,j,k}} - 10^{-\lambda_{i,j,g} d_{1gi,j,k}} \quad (\text{B-11})$$

$$\frac{\partial u}{\partial \lambda_l} = -m_{l_{i,j,g}} d_{2gi,j,k} 10^{-\lambda_{i,j,g} d_{2gi,j,k}} \ln 10 + m_{l_{i,j,g}} d_{1gi,j,k} 10^{-\lambda_{i,j,g} d_{1gi,j,k}} \ln 10 \quad (\text{B-12})$$

$$v = -\lambda_{i,j,g} (d_{2gi,j,k} - d_{1gi,j,k}) \ln 10 \quad (\text{B-13})$$

$$\frac{\partial v}{\partial \lambda_l} = -m_{l_{i,j,g}} (d_{2gi,j,k} - d_{1gi,j,k}) \ln 10 \quad (\text{B-14})$$

Using these equations, the derivative of transmissivity can be calculated and used to calculate the derivative of the horizontal conductances.

Derivative of Vertical Conductance with respect to a Depth-Dependence Parameter

When vertical anisotropy is used to define the vertical hydraulic conductivity, the vertical conductance also will be sensitive to a depth-dependence parameter. In this case, the vertical conductance is calculated as:

$$CV_{i,j,k+1/2} = \frac{\Delta r_j \Delta c_i}{\sum_{g=1}^n \left[\frac{thk_{g_{i,j,k+1/2}}}{\frac{M_{KDEP_{gi,j,k}} \sum_{l=1}^p Kh_l m_{l_{i,j,g}}}{VANI_g m_{gi,j}}} \right]} \quad (\text{B-15})$$

Because this is a complicated expression, it is useful to derive the sensitivity equation in several steps using equation B-10. First, the following definitions of u_l and v_l are assumed, which results in the derivatives shown:

$$u_l = thk_{g_{i,j,k+1/2}}; \quad \frac{\partial u_l}{\partial \lambda_l} = 0 \quad (\text{B-16})$$

$$v_1 = \frac{M_{KDEP_{g_{i,j,k}}} \sum_{l=1}^p Kh_l m_{l_{i,j,g}}}{VANI_g m_{g_{i,j}}}; \quad \frac{\partial v_1}{\partial \lambda_l} = \frac{\frac{\partial M_{KDEP_{g_{i,j,k}}}}{\partial \lambda_l} \sum_{l=1}^p Kh_l m_{l_{i,j,g}}}{VANI_g m_{g_{i,j}}} \quad (\text{B-17})$$

Then, using equation B-10,

$$\begin{aligned} \frac{\partial \sum_{g=1}^n \frac{u_1}{v_1}}{\partial \lambda_l} &= \sum_{g=1}^n \frac{\partial \frac{u_1}{v_1}}{\partial \lambda_l} = \sum_{g=1}^n \frac{-thk_{g_{i,j,k+1/2}} \frac{\frac{\partial M_{KDEP_{g_{i,j,k}}}}{\partial \lambda_l} \sum_{l=1}^p Kh_l m_{l_{i,j,g}}}{VANI_g m_{g_{i,j}}}}{\left(\frac{M_{KDEP_{g_{i,j,k}}} \sum_{l=1}^p Kh_l m_{l_{i,j,g}}}{VANI_g m_{g_{i,j}}} \right)^2} \\ &= \sum_{g=1}^n \frac{-thk_{g_{i,j,k+1/2}} \frac{\partial M_{KDEP_{g_{i,j,k}}}}{\partial \lambda_l}}{M_{KDEP_{g_{i,j,k}}}^2 \frac{\sum_{l=1}^p Kh_l m_{l_{i,j,g}}}{VANI_g m_{g_{i,j}}}} \end{aligned} \quad (\text{B-18})$$

Next, the following definitions of u_2 and v_2 are assumed,

$$u_2 = \Delta r_j \Delta c_i; \quad \frac{\partial u_2}{\partial \lambda_l} = 0 \quad (\text{B-19})$$

$$v_2 = \sum_{g=1}^n \frac{thk_{g_{i,j,k+1/2}}}{\frac{M_{KDEP_{g_{i,j,k}}} \sum_{l=1}^p Kh_l m_{l_{i,j,g}}}{VANI_g m_{g_{i,j}}}}; \quad \frac{\partial v_2}{\partial \lambda_l} = \frac{\frac{\partial u_1}{\partial v_1}}{\frac{\partial v_1}{\partial \lambda_l}}, \quad (\text{B-20})$$

which is shown in equation B-18. Then, using equation B-10,

$$\begin{aligned}
& -\Delta r_j \Delta c_i \sum_{g=1}^n \frac{-thk_{g_{i,j,k+1/2}}}{VANI_g m_{g_{i,j}}} \frac{\frac{\partial M_{KDEP_{g_{i,j,k}}}}{\partial \lambda_l} \sum_{l=1}^p Kh_l m_{l_{i,j,g}}}{VANI_g m_{g_{i,j}}} \\
\frac{\partial CV_{i,j,k+1/2}}{\partial \lambda_l} &= \frac{\left(\frac{M_{KDEP_{g_{i,j,k}}} \sum_{l=1}^p Kh_l m_{l_{i,j,g}}}{VANI_g m_{g_{i,j}}} \right)^2}{\left(\sum_{g=1}^n \frac{thk_{g_{i,j,k+1/2}}}{\frac{M_{KDEP_{g_{i,j,k}}} \sum_{l=1}^p Kh_l m_{l_{i,j,g}}}{VANI_g m_{g_{i,j}}}} \right)^2} \\
&= \frac{CV_{i,j,k+1/2}^2}{\Delta r_j \Delta c_i} \sum_{g=1}^n \frac{-thk_{g_{i,j,k+1/2}} \frac{\partial M_{KDEP_{g_{i,j,k}}}}{\partial \lambda_l}}{M_{KDEP_{g_{i,j,k}}}^2 \sum_{l=1}^p Kh_l m_{l_{i,j,g}}} \frac{1}{VANI_g m_{g_{i,j}}}
\end{aligned} \tag{B-21}$$