Improved Calculations for Dewatered Cells in MODFLOW

by John Doherty[1]

Abstract

Use of the United States Geological Survey ground water flow model MODFLOW is often hampered by the occurrence of "dry cells." While MODFLOW allows such cells to "rewet" in the course of a simulation, stability of the heads solution process is often problematical with rewetting functionality operative. In many cases of practical interest (particularly in mining applications), MODFLOW simply fails to converge. However by making a number of adjustments to the MODFLOW Block-Centered Flow package, it is possible to overcome this problem in many instances of MODFLOW deployment. These adjustments are such as to allow a layer to transmit water, albeit with a vastly reduced transmissivity, even if the water level in that layer is below its base. With these alterations MODFLOW cells can remain active even if they lie within the unsaturated zone.

Testing of the code has demonstrated its ability to perform well in situations where performance of the unmodified MODFLOW is degraded by the necessity to dry and rewet cells. Comparison of heads calculated using the modified MODFLOW with those calculated using MODFLOW-SURFACT (a MODFLOW-based code developed by HydroGeoLogic Inc. that prevents the occurrence of dry cells through use of pseudo soil functions) reveals near-identical results between the two codes. Comparison with analytical solutions of water table location also reveals near coincidence. An example of one such application is presented herein.

Introduction

One of the most frustrating aspects of working with MODFLOW, the modular, cell-centered, finite-difference ground water modeling program developed by the United States Geological Survey (McDonald and Harbaugh 1988) is the occurrence of "dry cells." A cell becomes "dry" when the calculated head in that cell falls below the base of the cell. When this occurs, MODFLOW immediately changes the status of the cell to inactive. The cell can later be "rewet" if water levels in neighboring cells are above user-defined thresholds.

There are many problems associated with the occurrence of dry cells, including:

- When a cell is declared as dry and thus made inactive, it can receive no external water. Thus recharge assigned to that cell through MODFLOW input files may never actually enter the ground water model domain. This phenomenon can be avoided to some extent in multilayer models by assigning recharge to the top active cell of the grid rather than to specific cells; however, if the bottom layer dries out, recharge is lost completely. The loss of recharge then promulgates the occurrence of dry cells in a kind of cascading effect.
- Operation of MODFLOW drying/rewetting functionality often leads to numerical instability. Most modelers have encountered cases where MODFLOW's solvers simply will not converge as cells in critical locations go dry and are then rewet on subsequent solution iterations. Attempts to facilitate solution convergence in the face of such oscillatory behavior by setting the solution convergence criterion unusually high often result in unacceptable budget errors. The iteration interval for attempting to rewet cells can also be set high to help overcome this problem; however, this can lead to questionable numerical solutions to the ground water flow equations.
- When MODFLOW calibration is undertaken using nonlinear parameter estimation software such as PEST (Doherty 1994), MODFLOWP (Hill 1992), UCODE (Poeter and Hill 1998), and MODFLOW 2000 (Harbaugh et al. 2000; Hill et al. 2000), the drying and rewetting of cells adds a degree of granularity to model outputs such that continuity of these outputs with respect to adjustable parameters is lost. This has a deleterious effect on the operation of the Gauss-Marquardt-Levenberg method on which these packages are based. Where observation bores are situated in dry cells the effect on the inversion process can be disastrous, as these cells are then assigned a spurious, but easily identified, head value by MODFLOW. While this effect can be mitigated somewhat by setting the heads of dry cells to the elevations of the bottoms of these cells, or by temporarily omitting affected observations from the inversion process, performance of the nonlinear parameter estimation process is nevertheless severely hampered.

The drying/rewetting problem can be particularly damaging when undertaking groundwater modeling for mining applications.

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While MODFLOW seems to be capable of simulating ground water flow in the vicinity of a pit that is gradually deepening, it often encounters difficulties in modeling ground water recovery following pit closure. The latter involves simulation of a rising water table and the progressive rewetting of upper layer cells. This is sometimes accompanied by extreme difficulty in solution convergence, no matter which MODFLOW solution package is employed.

This paper documents a methodology whereby the drying/rewetting problem can be overcome in certain situations through the introduction of a number of simple modifications to MODFLOW. Although, as is demonstrated herein, usage of the method so far has demonstrated applicability over a range of geological conditions, further testing over a much broader range of conditions is still required before the method can be generally accepted.

The Methodology

Horizontal Intercell Conductance

As is explained in McDonald and Harbaugh (1988), unconfined ground water flow can be simulated using a MODFLOW type 3 (i.e., confined/unconfined) or type 1 (unconfined) layer. When simulating unconfined conditions in either of these layer types, MODFLOW calculates the transmissivity at each cell center as the saturated thickness at the cell center multiplied by the hydraulic conductivity assigned to the cell. In formulating the finite difference flow matrix, horizontal intercell conductances are then computed by combining the transmissivities pertaining to neighboring cell centers in various ways, depending on flow conditions and on the manner in which hydraulic conductivity is assumed to vary between these cell centers (Goode and Appel 1992).

If the saturated thickness at any cell center becomes zero or negative in the course of the heads solution procedure for any MODFLOW time step, the offending cell is declared inactive and all intercell conductances associated with the cell are assigned the value of zero.

In the modified version of MODFLOW discussed herein, no cell is ever declared as dry. In order to accommodate the fact that water levels may fall below the base of a layer, the method of computing transmissivity at each cell center is altered slightly from that presently used by MODFLOW. In the normal MODFLOW, transmissivity is calculated using the formula

$$T = K(h - b) \tag{1}$$

where

T is the transmissivity at the cell center
K is the hydraulic conductivity assigned to the cell
h is the MODFLOW-calculated head in the cell
b is the elevation of the bottom of the cell.

In the modified MODFLOW, transmissivity is calculated using two equations: one applicable when the head is above the base of the cell, and the other applicable when the head is below the base of the cell. These equations are

$$T = Kt_r e^{-gt} + Kt \qquad \text{for } t > 0 \tag{2}$$

$$T = Kt_r e^{ft} \qquad \text{for } t < 0 \tag{3}$$

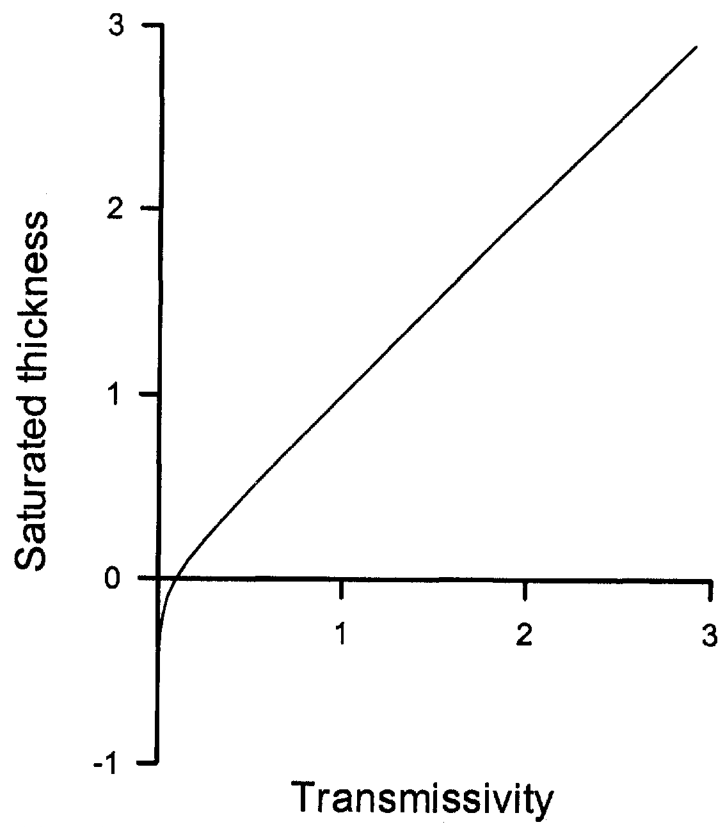

Figure 1. Transmissivity as a function of water level computed for a MODFLOW cell center; t_r = 0.1; f = 6.0; K = 1.0.

where

t is the saturated thickness, (i.e., h − b)
g, f are exponential decay coefficients
t_r is the residual saturated thickness.

Provided g is positive, the first term in Equation 2 decays to zero as the saturated thickness increases; hence, as long as the saturated thickness is not small, the transmissivity calculated using Equation 2 is the same as that calculated using Equation 1. However, as the saturated thickness is reduced, the transmissivity is not allowed to decay to zero. Rather, when the saturated thickness is zero, transmissivity is equal to Kt_r where t_r is the residual saturated thickness. Thus when the water level in the cell is equal to the elevation of the base of the cell, the transmissivity computed for the center of the cell is equal to that which would prevail if there were, in fact, a saturated thickness of t_r at the cell center rather than a saturated thickness of zero.

Once the calculated head falls below the base of the cell, transmissivity is computed using Equation 3. Transmissivity thus decays exponentially as the head falls further and further below the base of the layer. The higher is the value of f in this equation, the more rapid is the decay of transmissivity with decreasing h. Note that f must be positive.

To ensure that transmissivity calculated using Equations 2 and 3 is continuous and continuously differentiable as the head crosses the bottom of a MODFLOW layer, the following relationship must apply:

$$g = \frac{1}{t_r} - f \tag{4}$$

In implementing this methodology in the modified MODFLOW, the user selects a residual thickness t_r and an exponential decay rate f for Equation 3. The decay rate for the first term of Equation 2 (i.e., g) is then calculated using Equation 4. However, for this decay rate to be positive, as it must be if Equation 2 is to approach Equation 1 as the saturated thickness increases, the following condition must apply:

$$f < \frac{1}{t_r} \tag{5}$$

Figure 1 shows an example of the variation of transmissivity with saturated thickness calculated using Equations 2 and 3.

The methods by which intercell conductances are calculated from cell center transmissivities in the modified MODFLOW are unaltered from those described by Goode and Appel (1992).

Vertical Intercell Conductance

If, for a MODFLOW type 2 (confined/unconfined with constant transmissivity) or type 3 (confined/unconfined with variable transmissivity) layer, the head in a particular cell is below its top and the overlying cell is not inactive, MODFLOW supplies a correction to its normal vertical leakage term in formulating the finite-difference flow matrix. This correction is applied in order to simulate the fact that vertical flow between an upper active cell and a partially saturated underlying cell is driven by a head difference equal to the head in the overlying cell minus the elevation of the top of the underlying cell (rather than the actual head in the underlying cell).

Where a cell is declared dry because the water table falls below its base, the vertical leakage correction term is not applied in calculating flow to an underlying cell because no such flow can take place. However, if the cell is not declared dry in spite of the fact that the head in that cell is below its base (as occurs in the modified MODFLOW described herein), MODFLOW must be prevented from applying its vertical leackage correction as it is no longer required under these circumstances. If it is not prevented, MODFLOW will calculate flow from that cell to the underlying cell on the basis of a head difference that could actually lead to spurious flow reversals.

The modified version of MODFLOW allows the user two options for applying the vertical leakage correction term. The first option is to prevent the correction from being applied under any circumstances. This option is appropriate for three-dimensional simulation where a flow regime is modeled using a sequence of layers in which the elevation of the base of one layer is equal to the elevation of the top of the underlying layer. The second option, more appropriate for quasi-three-dimensional simulation where vertical intercell conductance accounts for the presence of an interlayer stratum of relatively low permeability, is to prevent the correction from being applied only when the head in the upper layer is below the base of that layer, thus preventing the occurrence of spurious flow reversals.

Variable Interlayer Conductance

In the normal MODFLOW, the elevation of the water table in any column of the grid is defined as the head in the highest active cell of that column (cells above the water table being rendered inactive by MODFLOW). For the modified MODFLOW, the elevation of the water table is defined as the head in the highest cell for which the MODFLOW-computed head is above the base of the respective layer. For cells higher than this, MODFLOW-calculated heads are below respective layer bottom elevations.

Because no cell is declared as dry, MODFLOW inputs such as recharge, and boundary conditions such as the river and general head boundaries, that exist in upper model layers are not rendered inoperative when the water table falls below these upper layers; in the case of river and head boundaries, this is a definite improvement over the operation of the normal MODFLOW as recharge from these sources would otherwise be completely lost. However, water moving from these boundaries to the water table must now move vertically though the interlayer conductances existing between the boundary and the water table. Where these interlayer conductances are low, the computed water table can suffer a discontinuity as it crosses a layer boundary due to the fact that water flowing to the ground water system from above the water table must do so through an extra interlayer conductance when the water table drops below the bottom of any layer, and hence must suffer a drop in head in the process.

To circumvent this occurrence the modified MODFLOW can increase interlayer conductance as the water table within a layer falls close to the bottom of that layer. This is done through introducing a linear reduction of interlayer resistance (reciprocal of conductance) with water table elevation within a layer, as long as the water table height is below a certain distance above the bottom of the layer. Mathematically this is described by the equations

$$R = R_u \qquad \text{for } h \geq h_u \tag{6}$$

$$R = R_b + \frac{(h - b)}{(h_u - b)}(R_u - R_b) \qquad \text{for } h_u > h > b \tag{7}$$

$$R = R_b \qquad \text{for } h \leq b \tag{8}$$

where

- R is the new interlayer resistance (reciprocal of conductance)
- h_u is the water level below which the linear decrease in R is activated (supplied by the user)
- b is the elevation of the base of the layer
- R_u is the interlayer resistance calculated as the reciprocal of the interlayer conductance used by the standard MODFLOW
- R_b is the interlayer resistance used by the modified MODFLOW when the water table is below the base of a layer.

R_b is calculated as the reciprocal of the "enhanced interlayer conductance," which is given by the equation

$$C_b = mC \tag{9}$$

where

- C is the interlayer conductance used by the standard MODFLOW
- m is a user-supplied multiplier for this conductance.

Through the operation of this mechanism, contact between the water table and external flow boundaries is maintained as the water table falls. Resistance to flow from any boundaries thus continues to be defined by the parameters that govern operation of the boundary, rather than by the length of the flowpath between the boundary and the water table. In many modeling contexts, this is a desirable feature. Where it is not, the user is free to leave intercell conductances independent of cell water level.

Cell Water Storage

MODFLOW calculates the change in stored water in any cell during any time step by multiplying the difference in the head computed for that cell between the beginning and end of that time step by the area of the cell and by an appropriate storage coefficient. For layers of type 2 and 3 (both of these being confined/unconfined layers) this storage coefficient is regarded as either "primary" or "secondary" depending on whether the head is above or below the top of the layer; in the latter case, the specific yield is the most appropriate storage coefficient to use.

When the water level falls below the bottom of a cell, however, it is no longer appropriate to calculate the change in stored water for the cell using the specific yield assigned to that cell; a much lower storage coefficient (possibly zero) is required under these circumstances. As part of the input dataset required by the modified MODFLOW, the user must supply an appropriate storage coefficient to use when a cell is "desaturated," i.e., when the water level in the cell is below its base.

The ability of the modified MODFLOW to switch to the use of a different storage coefficient as the head crosses the lower layer boundary is similar in many respects to its ability to switch between the use of a primary and secondary storage coefficient as the water table crosses the upper boundary of a confined/unconfined layer. Mathematically, the change in the amount of water stored in any cell between the beginning and end of a time step is calculated by integrating the product of head difference and storage coefficient between the old and new water level elevations for that time step and multiplying by the cell area. The storage coefficient along different segments of the integration path between the old and new head levels depends on whether each such segment lies within the current layer (where specific yield is employed), in an overlying layer (where primary storage coefficient is employed), or in an underlying layer (where the desaturated storage coefficient is employed).

Physical Significance of the Modifications

Although motivated by the need for numerical stability in the MODFLOW solution process, the modifications discussed herein do not constitute a contravention of reality. Under unsaturated conditions, movement of water within the subsurface can still take place, albeit with a vastly diminished hydraulic conductivity and with much smaller changes to volumetric water storage than what would take place under saturated flow conditions.

The functional dependence of layer transmissivity on head described by Equations 2 and 3 can also be considered to reflect the fact that the elevation of the bottom of a cell is unlikely to be uniform through the entirety of that cell. Thus there is a "residual transmissivity" when the calculated head is equal to the notional bottom of the cell; transmissivity then decays quickly as the head falls below the notional layer base. This concept of transmissivity is just as much in harmony with reality as the concept of a strictly linear transmissivity variation that decays to exactly zero at the notional layer bottom.

A description of transmissivity based on Equations 2 and 3 can also be used to represent the situation in which a small amount of flow takes place beneath the base of the model domain—a not uncommon occurrence. If the lowest model layer is assigned a transmissivity decay rate (i.e., f) of zero, then no matter how far below the base of the lowest layer the water table lies, the transmissivity computed for cells in this lowest layer never falls below Kt_r, (i.e., the hydraulic conductivity of the lowest layer times the residual saturated thickness assigned to that layer). This simulates the fact that rocks which underlie a recognized aquifer may indeed conduct water, although not as readily as those that make up the aquifer itself.

It can also be argued that the transmissivity function represented by Equations 2 and 3 is unlikely to be any more of a contravention of reality than the myriad of other assumptions that must be invoked to simulate a complex environmental system by a numerical model. These include the assumptions of cell property uniformity or of linear intercell property variation that formulations of intercell conductance are based on. Other assumptions are invoked "by the bucketful" when various zonations, or other simplifying descriptions of distributed parameter distribution, are introduced to the model domain as part of the calibration process.

The functional dependence of the vertical conductance between two model layers on the head in the upper layer is in harmony with the fact that when the water table in a cell is low, the average flowpath for water between that cell and the underlying cell is less than when the cell is full. Hence the average conductance associated with this path should increase with diminished water depth.

Selection of Parameter Values

Use of the methodology described herein for the handling of desaturated conditions within MODFLOW requires that the user supply values for a number of variables that are not required by the normal MODFLOW. Specifically, values are required for the residual thickness t_r, the transmissivity decay rate f, the desaturated storage coefficient, the vertical conductance multiplier, and the vertical elevation at which the linear decrease of interlayer resistance is activated.

Ideally t_r should be set as low as possible and f set as high as possible so that, with minimal residual saturated thickness and a high rate of decay of desaturated transmissivity, intercell conductances under desaturated conditions are very low. For a given t_r the upper limit of f is set by Equation 5; on most occasions f should be set just below this upper limit. Hence the user is effectively required to select just one parameter (i.e., t_r) for implementation of the methodology described herein in a particular modeling context. It has been found that if t_r is set too low numerical instability can occur, resulting in failure of the MODFLOW iterative solution process. The onset of this instability thus sets the lower limit for this parameter.

Experience in many different modeling contexts has demonstrated that if t_r is not set so low as to induce numerical instability, and if f is calculated so as to just satisfy Equation 5, MODFLOW-calculated heads and flows are quite insensitive to t_r over a broad range of values for this variable (generally over at least an order of magnitude). The value that should be assigned to t_r is case-specific. However, as a rule of thumb, a value for t_r of between 1% and 5% of the layer thickness works well in most cases. As the following example demonstrates, deviations from the "true" solutions to the ground water flow equations when values for t_r and f are selected in this manner are mostly very small indeed (smaller, often, than deviations that result from operation of MODFLOW's drying/rewetting functionality, the use of which also requires that values for a number of somewhat arbitrary variables be selected).

Naturally, if t_r is set too high and/or if f is set too low, erroneous solutions to the flow equations may result from the artificially elevated intercell conductances that prevail under these conditions. This will be especially true if underlying layers are relatively nonconin the cell lies between the upper and lower adjustment levels, the pumping rate is derated linearly in proportion to the distance of the water table below the upper adjustment level. If the water table is at or below the lower adjustment level, the pumping rate from the bore is zero.

In practice, the lower adjustment level for a particular bore should be situated at the base of the borehole's screened interval. The distance between the lower and upper adjustment levels should be set at the cell-to-borehole correction at full pumping rate (Lerner 1989; Anderson and Woessner 1992). In this manner, a bore can pump at its rated level until the water table at the actual bore (i.e., the MODFLOW-calculated water level for the cell minus the cell-to-bore correction) has fallen to the bottom of the screened interval. Because the bore-to-cell correction does not deviate too far from linearity, the methodology described herein then has the effect of maintaining the water table at the bore at a level no lower than the base of the screen by automatically varying its pumping rate to ensure that this occurs.

An Example

Description

Figure 2 shows a finite difference grid comprising 50 cells in each of the row and column directions; each cell is 100 m × 100 m in areal extent. The model is three layers deep, each layer being 25 m in height. The model has a fixed head boundary running along both its left and right margins. Along the right edge the boundary head is set at 70 m, i.e., 20 m above the bottom of the top model layer. Heads along the left boundary are fixed at an elevation of 5 m above the base of the lowest layer; fixed head cells are deployed only in the lowest MODFLOW layer along this left boundary of the grid. Except for the fixed head boundary at the left of the system, initial heads are everywhere 70 m.

Horizontal and vertical hydraulic conductivity is everywhere 1 m/day. Specific storage is uniformly 10^{-5} while specific yield is 0.1. Recharge (applied to the top active layer) is 1×10^{-4} m/day.

At a time of zero days a rectangular drain with an elevation of 10 m and a conductance of 1000 m^2/day is inserted in the bottom layer; see Figure 2 for its location. It is maintained in this position for 1000 days (simulated by 10 MODFLOW time steps using a time step length multiplier of 1.2). During this time heads within the model domain respond to stresses imposed from two sources, these being (a) the imposition of the drains, and (b) the fact that initial heads are not in balance with the fixed heads situated at either end of the model domain and with recharge. After 1000 days the drains are removed. Recovery of water levels is then simulated by a single MODFLOW stress period of 2000 days made up of 20 time steps with a time step length multiplier of 1.2.

It is acknowledged that this model is a little artificial in that initial ground water levels are far removed from equilibrium with model recharge and boundary conditions. This was purposefully done to "test" the new functionality, requiring that the model respond rapidly to the imposed boundary conditions with a water table that falls quickly across layer boundaries, resulting in widespread desaturation of upper layer cells.

Numerical Simulation

All layers were assigned a LAYCON value of 13. That is, each layer was designated as a MODFLOW type 3 (confined/unconfined) layer, allowing transmissivity dependence on water level up to an elevation equal to the top of the layer, with intercell conductance calculated using arithmetic averaging (the most appropriate averaging method where flow is unconfined and recharge is small or zero). Using a residual thickness (i.e., t_r from Equations 2 and 3) of 0.1 m and a decay constant (i.e., f from Equation 3) of 6 m for all three model layers, the model was run over both stress periods using the PCG2 solution package with a head convergence criterion of 1×10^{-4} m. (Note that model outputs are virtually insensitive to t_r and f at these values; note also that no head-dependent adjustment was made to vertical interlayer conductance in this simulation.) The model ran to the end of the simulation without experiencing any difficulties; mass balance error was less than 0.01%. Figure 3 shows the water table calculated by the modified MODFLOW for the end of stress period 1 as a solid line. Figure 4 (upper solid line) shows the water table profile calculated by the modified MODFLOW for the end of stress period 2, i.e., at 2000 days after removal of the drains.

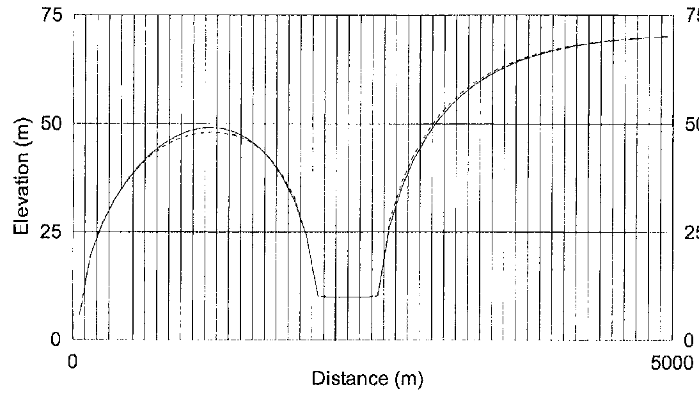

Figure 3. Water table at the end of stress period 1 calculated using the modified MODFLOW (solid line) and the unmodified MODFLOW (dashed line).

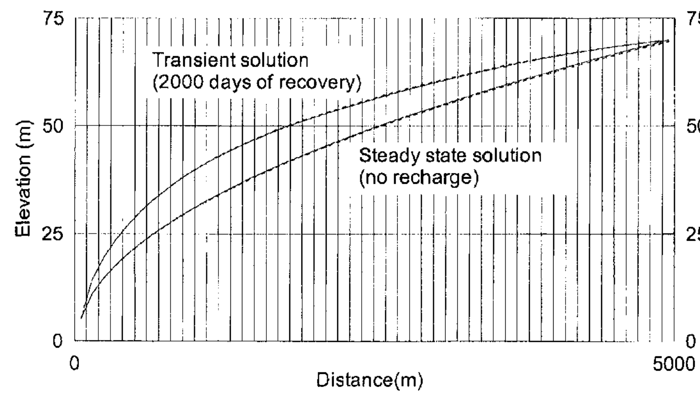

Figure 4. Water table calculated using the modified MODFLOW (upper solid line) and the unmodified MODFLOW (upper dashed line) after a recovery period of 2000 days. Also shown is the water table calculated under steady-state conditions by the modified MODFLOW (lower solid line) together with an analytical solution (lower dashed line).

Water levels calculated by the unmodified MODFLOW are shown as a dashed line in Figure 3 and in the upper curve of Figure 4. Solution convergence could not be attained during the rewetting phase unless MODFLOW rewetting settings were such that cells could be rewet only from below. The wetting threshold was set at 0.1 m with rewetted heads calculated using the equation

$$h = BOT + WETFCT\ (hn - BOT)$$

with WETFCT set to 1.0 (McDonald et al. 1991).

ductive. By applying Equations 2 and 3 (particularly 3) to calculate the amount of desaturated transmissivity that is induced by the modifications described herein, and by comparing this with the transmissivity of underlying layers, it will quickly become apparent whether the use of particular values for t_r and f will result in too large a deviation from ideal conditions. If, for a particular problem, t_r cannot be lowered sufficiently and f cannot be raised sufficiently to reduce desaturated transmissivity to a suitably low level without the onset of numerical instability, then the modifications described herein may not be suitable for that particular problem.

The value selected for desaturated storage coefficient is a matter of user preference, for stability of the methodology described herein does not depend on it. Under most circumstances it should be set to zero, indicating that unsaturated zone storage plays little or no part in the characterization of the flow regime. However, as mentioned, there may be situations where a nonzero value for this variable is preferred.

The use of a variable interlayer resistance is also a matter of user preference; it has no bearing on the stability or otherwise of the MODFLOW heads solution process under desaturated conditions. Implementation of this functionality allows lower layers to receive recharge waters from above just as easily when the water table is low, as when it is high. This is what MODFLOW does when it assigns recharge to the top active layer of the model, thereby bypassing any overlying dry cells. (This is conceptually equivalent to assigning the interlayer conductance of these dry cells a value equal to infinity). By increasing interlayer conductance as a cell becomes desaturated, the user has the option of replicating this behavior in the modified MODFLOW, where the layer recharge is assigned to does not change as the water table fluctuates. If implementation of this functionality is not warranted in a particular modeling context, then the interlayer conductance can be left unchanged.

Recognition of Desaturated Cells

In the normal MODFLOW a special, user-assigned head value is assigned to cells that are declared dry. Such cells are then easily recognized by postprocessing software. Where such software is used to display MODFLOW results, the status of such cells can be made readily apparent by appropriate choice of color. Where a MODFLOW postprocessor is used to undertake spatial interpolation of MODFLOW-calculated heads at grid cell centers to the sites of observation bores for comparison with field measurements, use of the dummy head value allows the action of the postprocessor to be modified where one or more of the cells involved in the spatial interpolation process become dry.

In the modified MODFLOW, desaturated cells still take part in the heads calculation process because no such cells are declared inactive. Heads in desaturated cells affect the heads calculated for neighboring saturated and desaturated cells through the horizontal and vertical conductance linkages that still exist between them. Hence heads in desaturated cells cannot be altered to a value that signifies their desaturated condition. Thus desaturated cells must be recognized in MODFLOW postprocessing software as cells in which the head is below the base of the respective layer.

If postprocessing is undertaken for the purpose of interpolating MODFLOW heads to the sites of bores for comparison with measured water levels, and if such comparisons are used to guide the direction of a parameter estimation process such as that undertaken by PEST, UCODE, or MODFLOW 2000, the occurrence of

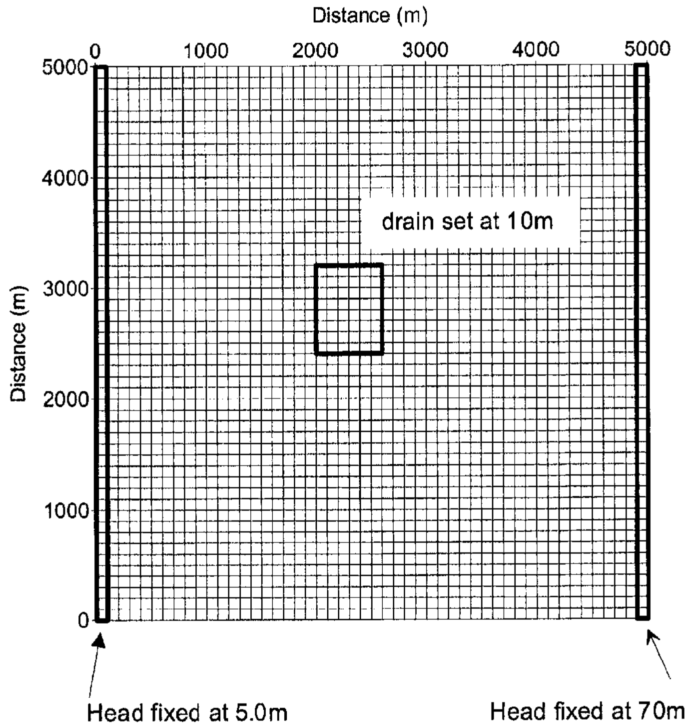

Figure 2. Model grid showing drains and fixed head boundaries.

desaturation in measurement cells can be treated in a variety of ways. Theoretically, the modified MODFLOW maintains continuity of heads with respect to parameter values even where cells are desaturated; hence, model-generated heads affected by desaturation can still be used as part of the parameter estimation process, even where corresponding measured heads show saturated conditions. The "pull" exerted by the model-to-measurement discrepancy should assist in the determination of a set of parameters that return the affected cells to saturation. However, in using the modified MODFLOW so far, incidences have been noted where desaturation of upper layers can lead to heads which show some slight discontinuity with respect to parameter values in those layers. Such conditions are most likely to occur where recharge, or any upper layer inflow boundary condition, is absent; in such cases there is no downward flow of water to enforce a calculable head gradient between upper cells and the water table, a situation which is compounded by the low-conductance linkages between desaturated cells. Under such circumstances, it may be best to temporarily remove model-generated desaturated heads for which there are saturated field counterparts from the inversion process.

Automatic Pumping Rate Adjustment

As a complement to the changes made to MODFLOW that allow it to better handle desaturated conditions, the manner in which MODFLOW simulates pumping from a bore has also been enhanced. In the modified MODFLOW, the user can specify that the pumping rate from any bore be reduced automatically as the water table falls, such that pumping from the bore ceases altogether when the water level in the cell containing the bore falls to a certain level, specific to each bore. The user supplies an "upper adjustment level" and a "lower adjustment level" for each pumped bore. As long as the water level in the cell containing a bore is greater than the upper adjustment level, pumping from that bore takes place at the rate originally assigned by the user. When the water level

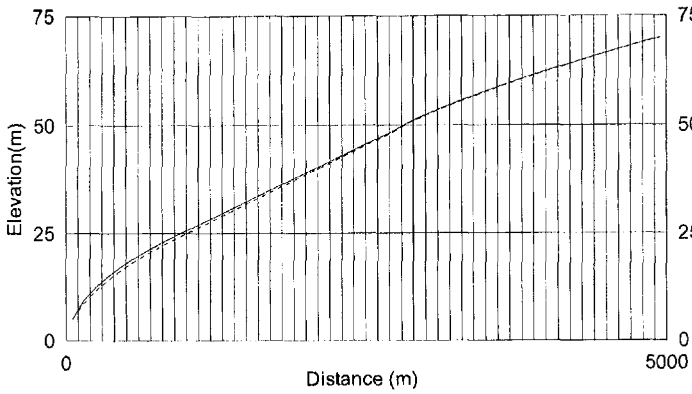

Figure 5. Steady-state water table calculated using the modified MODFLOW (solid line) and MODFLOW-SURFACT (dashed line) for low-conductivity middle layer and starting heads of 5 m.

Water levels calculated by the unmodified MODFLOW are nearly coincident with those calculated by the modified MODFLOW in Figure 4. However, it should be noted that the unmodified MODFLOW showed a perched water table situated in layer 2 in the first column of the model domain; this perched water table is not represented in either of Figures 3 or 4. Perching was due to the fact that during the iterative solution process, layer 3 quickly became unconfined in the fixed head cells along the left model boundary while layer 2 cells remained wet. Once this happened, the effect of the MODFLOW vertical leakage correction reduced the head differential driving flow of water between the second and third layers, thus maintaining wetness in layer 2 cells. Although this situation is undesirable, it did not result in incorrect heads elsewhere and, if recognized, can easily be accommodated in water level plots such as those shown in Figures 3 and 4 by representing the head in the lower layer rather than in the perched layer. However in other situations this problem may not have been so easily recognized.

As a check on the heads computed by the modified MODFLOW, this case was also run using MODFLOW-SURFACT (HydroGeoLogic 1996). MODFLOW-SURFACT overcomes MODFLOW drying-rewetting problems through the use of "pseudo soil functions" or, if desired, full simulation of variably saturated flow. Water level plots produced by MODFLOW-SURFACT are not distinguishable from those produced by the modified MODFLOW for either of Figures 3 and 4. Execution time on a 550 MHz Pentium 3 was 12.5 seconds for the modified MODFLOW and 28 seconds for MODFLOW-SURFACT using pseudo soil relations and its PCG4 solver with Newton-Raphson linearization. It is important to note that comparison of computation times for a single small model cannot constitute the basis for ranking the relative efficiency of the two codes. Nevertheless, from this and other tests undertaken to date, a comparison of execution speed of the modified MODFLOW with that of MODFLOW-SURFACT consistently reveals that the modified MODFLOW documented herein is as fast (often slightly faster) than MODFLOW-SURFACT.

A steady-state run was undertaken in order to determine water levels throughout the model domain under the assumption of zero vertical recharge. Figure 4 (lower solid line) represents water levels calculated by the modified MODFLOW. An analytical solution based on the Dupuit-Forscheimer assumption of horizontal ground water flow is represented by the corresponding dashed line. The two curves are almost coincident. (The near-coincidence of the two curves under conditions of zero recharge where the drains have been removed should not be construed as evidence that multiple layers are not required for simulation of this ground water system. The three-dimensional nature of ground water flow becomes more important when the drains are in place. Furthermore, its significance heightens if issues such as solute transport are to be examined with the model.)

As a variation of this test case, the hydraulic conductivity of the middle model layer was reduced from 1m/day to 0.01 m/day. Also, the initial water level was set uniformly to 5 m throughout the model domain, thus requiring that the water table move through the nonconductive and desaturated middle layer over much of the model domain in order to reach its equilibrium position. The steady-state water table profile computed by the modified MODFLOW is shown in Figure 5 as a solid line. Also shown is the water table profile computed by MODFLOW-SURFACT under identical conditions. It can be seen that the curves are almost coincident. Run times for the two models were also almost identical (about four seconds on a 550 MHz Pentium 3 machine).

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Editor's Note: The use of brand names in peer-reviewed papers is for identification purposes only and does not constitute endorsement by the authors, their employers, or the National Ground Water Association.

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