Adapting MODFLOW to Simulate Water Movement in the Unsaturated Zone

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ABSTRACT

We have adapted MODFLOW to incorporate soil moisture accounting, in order to quantify soil moisture storage and depletion above the water table. This capability is implemented through a new package for MODFLOW, the Vadose module. When this package is utilized, MODFLOW simulates flux within both the saturated and unsaturated zones using the van Genuchten relationships (van Genuchten, 1980) to define conditions in the unsaturated zone. The Rawls and Brakensiek empirical model (1989) is used to estimate hydraulic conductivity, specific retention, bubbling pressure and pressure-saturation curves for the assigned soil texture class of each model cell. Using the Rawls and Brakensiek-- identified hydraulic properties and the van Genuchten relationships, cells where unsaturated conditions occur are assigned a transmissivity and specific moisture capacity based on fluid pressure conditions within the cell. These parameters are used by MODFLOW in place of saturated transmissivity and storage coefficients to calculate fluid pressure/ head and movement of water between the unsaturated and saturated zone. Under these conditions, the occurrence of deep percolation to layers representing the saturated zone is delayed or reduced until soil moisture deficits have been satisfied from available recharge. Similarly, evapotranspiration utilizes available soil moisture before removing water from deeper saturated zones. Separate accounting for evapotranspiration from groundwater and from the vadose zone is automatically printed out as part of the MODFLOW flow budget.

INTRODUCTION

Accounting for soil moisture use in the unsaturated zone is often important to realistically simulating the delivery of recharge through the unsaturated zone to groundwater and enabling the simulation of the interaction of plants and the surface water – groundwater regime. While other programs are available to simulate fluid flow in variably saturated porous media (Hsieh, et.al, 2000), we were unable to find a model that works with MODFLOW, and uses the type of geologic information typically available, to model both saturated and unsaturated zone flow. This paper presents a way to enable MODFLOW to account for soil moisture in the vadose zone and allow the movement of water into and out of that zone.

A number of relationships have been published which link unsaturated hydrologic properties to total head (Brooks and Corey (1964), Haverkamp (1977), van Genuchten (1980)). We have chosen to use the Van Genuchten (1980) approximation of relative conductivity and soil water retention in the unsaturated zone to program a vadose module for MODFLOW. This module works with the existing budget accounting module of MODFLOW to track the movement of moisture between the unsaturated zone, the saturated zone, and evapotranspiration. This paper describes how the Vadose module works and presents several test cases to illustrate the results of using the Vadose module.

VADOSE MODULE FOR MODFLOW

Within the Vadose module, unsaturated cells are assigned an unsaturated relative transmissivity and specific moisture capacity based on saturated properties and a geologic characterization of the soil. The unsaturated parameters are used by MODFLOW in place of saturated transmissivity and storage coefficients, in conjunction with the pressure head in the unsaturated cells to calculate movement of water between the unsaturated and the saturated zone, and the amount of soil moisture in each layer of the unsaturated zone. Evapotranspiration demand is met to the extent possible by soil moisture, starting in the top cell and continuing down, until a saturated cell is encountered, or the depth of the cell center is below the extinction depth. If the saturated cell is above the extinction depth, the remaining ET need is met by groundwater.

Incorporation of the Vadose Module into MODFLOW

The Vadose module is incorporated into MODFLOW in a manner identical to the existing MODFLOW modules; its use involves indicating in the MODFLOW basic package input IUNIT(35) which unit to find input on, creation of one input file for the module, and running of the standard MODFLOW model which has been compiled with the Vadose module and a version of the MODFLOW main incorporating minor changes to call the Vadose module's subroutines. No changes are required to any other existing MODFLOW modules.

Van Genuchten Equation to calculate effective saturation [Equation 1a]

$$\frac{\theta - \theta_r}{\phi - \theta_r} = \left[\frac{1}{1 + (\alpha\psi)^n}\right]^m = SE$$

where $\theta =$ water content, $\theta_{\mathrm{r}} =$ residual water content,
$\phi =$ porosity,
$\alpha =$ constant $= y_b - 1,$
$n =$ constant $= \lambda + 1,$
$m =$ constant $= 1 - \dfrac{1}{\lambda + 1},$
$\lambda =$ pore size distribution index,
$y_b =$ bubbling pressure
$\psi =$ pressure head $= h\text{-}z, h =$ total hydraulic head,
$z =$ elevation head, and $SE =$ effective saturation

Input for the Vadose Module

The Vadose module input consists of: factors to convert centimeters and hours to model units, minimum soil pressure to which the plants can extract moisture, and the elevation of the top of layer one. For each layer, additional data required includes arrays of percent clay, percent sand, porosity, ratio of vertical to horizontal conductivity, either the elevation of the bottom of the layer or the layer thickness, and the initial soil moisture of that layer.

Van Genuchten Equation to calculate total head [Equation 1b]

$$h = -\left[\frac{1}{SE^{1/m}} - 1\right]^{1/n} + z$$

where $h =$ total hydraulic head, $SE =$ effective saturation,
$m =$ constant, $n =$ constant, and $z =$ elevation head

Initial Calculations

At the beginning of the simulation, the Vadose module uses the van Genuchten (1980) soil water retention and hydraulic conductivity functions, (Equations 1a, 1b and 2) to estimate partially saturated hydraulic conductivity and the effective saturation for the initial head and capillary pressure distribution. The van Genuchten equations require input parameters alpha , 'n', and 'm', which are based on soil properties. In this module if alpha, n, and m, are known, they can be specified. If they are not known, they are calculated by using the equations of Rawls and Brakensiek (1989).

Van Genuchten approximation of relative hydraulic conductivity [Equation 2]

$$\frac{K(\theta)}{K_{sat}} = \left(\frac{\theta - \theta_r}{\phi - \theta_r}\right)^{1/2}\left[1 - \left(1 - \left(\frac{\theta - \theta_r}{\phi - \theta_r}\right)^{1/m}\right)^m\right]$$

where $K(\theta) =$ relative hydraulic conductivity,
$K_{sat} =$ saturated hydraulic conductivity,
$\theta =$ water content, $\theta_{\mathrm{r}} =$ residual water content,
$\phi =$ porosity, $\alpha =$ constant, $n =$ constant, $m =$ constant

The Rawls and Brakensiek (1989) regression equations shown on Table 1 were developed by statistically correlating soils of known textures to soil-moisture curves as defined by the van Genuchten (1980) and Brooks-Corey (1964) models. These regression equations are used in this module to calculate bubbling pressure, Brooks-Corey pore size distribution index, Brooks-Corey residual water content, and saturated hydraulic conductivity to estimate input parameters alpha, ‘n’, and ‘m’ for the van Genuchten functions.

The calculated saturated transmissivity is used in the model whenever a cell becomes saturated. The program also calculates initial vertical transmissivity using the harmonic mean of calculated saturated transmissivities. Based on the van Genuchten approximation of effective saturation [Equation 1a], the program uses the initial soil moisture to calculate initial head values [Equation 1b] for unsaturated layers.

Table 1: Rawls and Brakensiek (1989) Regression Equations

$$\begin{aligned}
y_b = \; & \exp(5.3396738 + 0.1845038*PC - 2.48394546*\phi - 0.00213853*PC^2 - 0.04356349* \\
& PS*\phi - 0.61745089*PC*\phi + 0.00143598\ *PS^2*\phi^2 - 0.00855375*PC^2*\phi^2 - 0.00001282* \\
& PS^2*PC + 0.00895359*PC^2*\phi - 0.00072472*PS^2*\phi + 0.0000054*PC^2*PS + \\
& 0.50028060*\phi^2*PC)
\end{aligned}$$

$$\begin{aligned}
\lambda = \exp(& -0.7842831 + 0.0177544*PS - 1.062498*\phi - 0.00005304*PS^2 - 0.00273493*PC^2 + \\
& 1.11134946*\phi^2 - 0.03088295*PS*\phi + 0.00026587*PS^2*\phi^2 - 0.00610522*PC^2* \\
& \phi^2 - 0.00000235*PS^2*PC + 0.00798746*PC^2*\phi)
\end{aligned}$$

$$\begin{aligned}
\theta_r = \; & -0.0182482 + 0.00087269*PS + 0.00513488*PC + 0.02939286*\phi - 0.00015395*PC^2 - \\
& 0.0010827*PS*\phi - 0.00018233*PC^2*\phi^2 + 0.00030703*PC^2*\phi - 0.0023584*\phi^2*PC
\end{aligned}$$

$$\begin{aligned}
K_{sat} = \exp(& 19.52348*\phi - 8.96847 - 0.028212*PC + 0.00018107*PS - 0.0094125*PC^2 - \\
& 8.395215*\phi^2 + 0.077718*PS*\phi - 0.00298*PS^2*\phi^2 - 0.019492*PC^2*\phi^2 + \\
& 0.0000173*PS^2*PC + 0.02733*PC^2*\phi + 0.001434*PS^2*\phi - 0.0000035*PC^2*PS
\end{aligned}$$

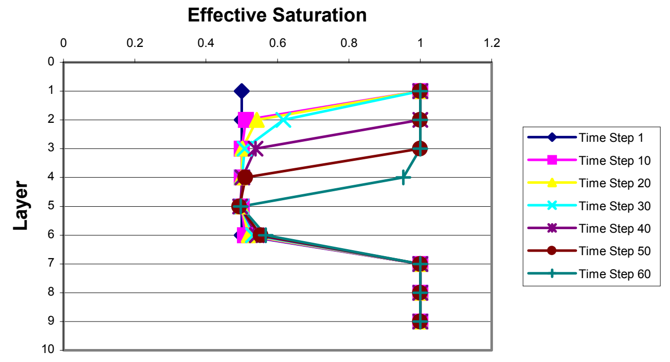
where y_b = bubbling pressure (cm)
λ = pore size distribution index
θ_r = residual moisture content
PC = percent clay
PS = percent sand
ϕ = porosity

Calculations for Each Time Step

For each time step, for all cells, the program calculates effective saturation based on heads from the previous time step. To determine the amount of soil moisture used from each unsaturated layer to satisfy evapotranspiration demand, the program uses the specified maximum evapotranspiration rate specified in the evapotranspiration package for that time step, the specified extinction depth, the calculated effective saturation, and the specified minimum pressure to which plants can remove soil moisture. Evapotranspiration demand is met to the extent possible by soil moisture, starting in the top cell and continuing down, until a saturated cell is encountered, or the depth of the cell center is below the extinction depth. If the saturated cell is above the extinction depth, the remaining evapotranspiration need is met by groundwater.

After soil moisture has been removed to satisfy evapotranspiration needs, the program recalculates effective saturation in each layer. The value of remaining soil moisture is used to calculate new values of head in unsaturated layers. Van Genuchten equations 1 and 2 are then used to calculate the relative transmissivity of the unsaturated layers and their specific moisture capacity, and the change in moisture for the calculated change in head. The unsaturated transmissivity is also used to calculate VCONT and branch conductances for the unsaturated zone cells. These values of branch conductances and VCONT are used within MODFLOW in a manner identical to the manner in which saturated transmissivity is used to calculate flow. Finally, the Vadose module calculates a volumetric budget for evapotranspiration from groundwater and from the vadose zone.

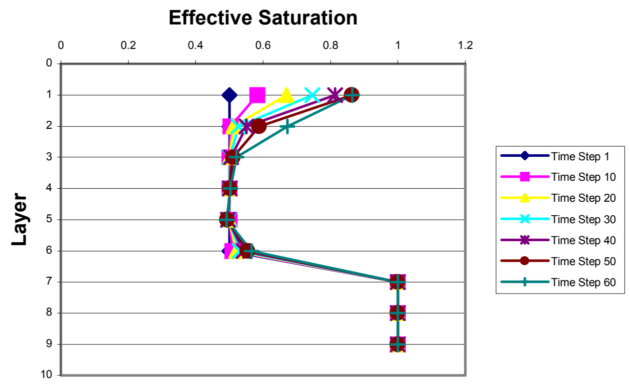
Figure 1: Test Case 1a, Recharge=0.3 ft/day, Zero ET



MODEL TEST CASES

Several simple test cases have been run to illustrate the workings of the Vadose module. The first series of test cases models a system with no evapotranspiration. They are designed to demonstrate how the Vadose module simulates the movement of the wetting front. The second type of test case includes evapotranspiration with no recharge and demonstrates the model's simulation of the interaction of plants with the unsaturated zone.

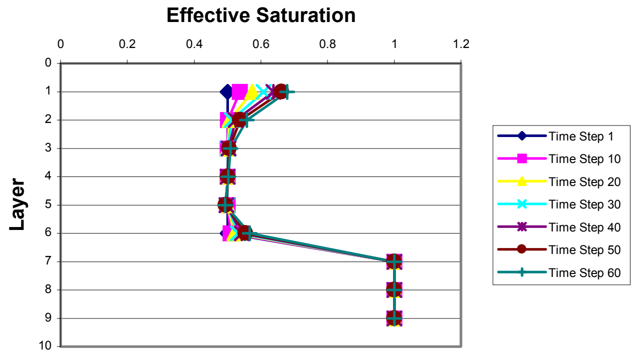
Figure 2: Test Case 1b, Recharge = 0.04 ft/day, Zero ET



Setup of Series 1 Test Cases – Recharge Only – No Evapotranspiration

The first series of test cases developed and presented here illustrate the capability of the Vadose module to simulate the movement of a wetting front in the vadose zone under constant recharge conditions. The framework of the test case is a homogenous grid consisting of nine 5-foot thick layers, each 5 X 5 cells. The grid begins with 50% saturation in the top six layers and maintains 100% saturation in the bottom three, thereby simulating an unsaturated zone underlain by a constant water table. The starting head in all cells is 20 feet.

Figure 3: Test Case 1c, Recharge = 0.02 ft/day, Zero ET



Saturated hydraulic properties and van Genuchten parameters were calculated using the Rawls and Brakensiek equations and the van Genuchten approximations based on model geology composed of 5% clay and 79% sand. The porosity was set at 0.435 and the specific yield to 0.00010. The ratio of vertical to horizontal hydraulic conductivity was set to 0.1.

These illustrative cases were run as transient simulations with one 30-day stress period broken up into 60 equal time steps. The grid was subjected to constant recharge in the top layer and no evapotranspiration. In test cases 1a, 1b, and 1c, recharge was set to 0.3 ft/day, 0.04 ft/day, and 0.02 ft/day, respectively.

Results of Series 1 Test Cases

As expected, the model results, shown in Figures 1-3, illustrate a wetting front moving through the vadose zone above a water table. Test Case 1a, illustrated in Figure 1, was run with a recharge rate of 0.3 ft/day. This saturated the top layer of the model by the 10th time step, and this saturated front moved progressively toward the water table, as expected. Similar results are shown for lower recharge rates in Test Cases 1b and 1c. Neither of these cases reached 100% saturation, but the motion of the unsaturated "front" can be seen in Figures 2 and 3.

Setup of Test Case 2 – Evapotranspiration Only

The second series of test cases developed and presented here illustrate the capabilities of the Vadose module to represent evapotranspiration (ET). The grid is identical to the one used for the first series of test cases. In Test Case 2, moisture is allowed to be withdrawn from the unsaturated zone to satisfy ET demands. In each time step, soil moisture is extracted to a minimum pressure of 0.5 milliPascals. This illustrative case was also run as a transient simulation with one 30-day stress period, divided into 60 equal time steps.

Figure 4: Test Case 2, Evapotranspiration = 1.0 ft/day, Zero Recharge

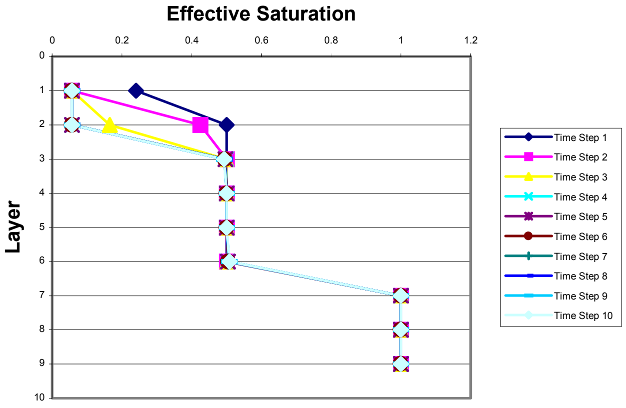
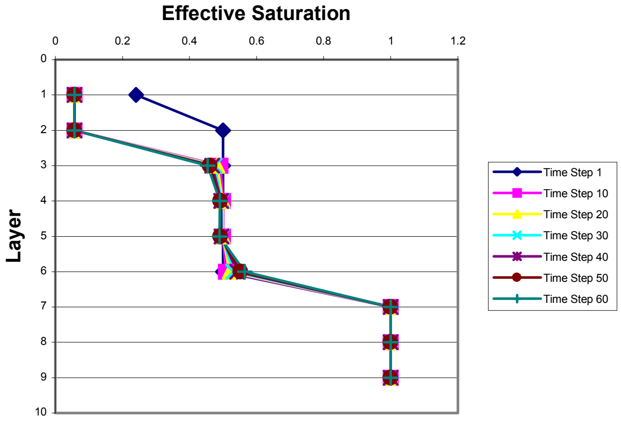


Figure 5: Test Case 2, Evapotranspiration = 1.0 ft/day, Zero Recharge



Results of Test Case 2

As shown in Figures 4 and 5, the soil moisture in the top layers of Test Case 2 decreases as ET extracts moisture from the unsaturated zone. It can be seen in Figure 4 that once the moisture has been depleted from Layer 1, the model looks to Layer 2 to satisfy ET demand, and so on. This illustrates the module's ability to model the physical relationship between ET demand and the unsaturated zone. Another feature of the module is the capability to show information on the volume and rate of ET in the overall model budget. Over time, the model looks deeper for soil moisture to satisfy ET (Figure 5), and the budget (Table 2) reflects the amount of water removed to satisfy that demand as well as the ET rate for the time step.

CONCLUSIONS

Review of the results from the model test cases indicate that this method of simulating movement of soil moisture through the unsaturated zone does behave as one would expect. With the addition of recharge

TABLE 2

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 VOLUMETRIC BUDGET FOR ENTIRE MODEL AT END OF TIME STEP 60 IN STRESS PERIOD  1
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    CUMULATIVE VOLUMES      L**3       RATES FOR THIS TIME STEP      L**3/T
    ------------------                 ------------------------

          IN:                                   IN:
          ---                                   ---
            STORAGE =         81.0329             STORAGE =          2.9592
      CONSTANT HEAD =          0.0000       CONSTANT HEAD =          0.0000
   ET FROM GRNDWATR =          0.0000    ET FROM GRNDWATR =          0.0000
   ET FROM SOIL MOI =          0.0000    ET FROM SOIL MOI =          0.0000
   STORAGE/SOIL MOI =       1068.3367    STORAGE/SOIL MOI =      7.2020E-05
           RECHARGE =          0.0000            RECHARGE =          0.0000

           TOTAL IN =       1149.3695            TOTAL IN =          2.9593

         OUT:                                  OUT:
         ----                                  ----
            STORAGE =         80.2169             STORAGE =          2.9377
      CONSTANT HEAD =          0.0000       CONSTANT HEAD =          0.0000
   ET FROM GRNDWATR =          0.0000    ET FROM GRNDWATR =          0.0000
   ET FROM SOIL MOI =       1068.3367    ET FROM SOIL MOI =      7.2020E-05
   STORAGE/SOIL MOI =          0.0000    STORAGE/SOIL MOI =          0.0000
           RECHARGE =          0.0000            RECHARGE =          0.0000

          TOTAL OUT =       1148.5536           TOTAL OUT =          2.9378

           IN - OUT =          0.8159            IN - OUT =      2.1476E-02

PERCENT DISCREPANCY =            0.07  PERCENT DISCREPANCY =            0.73
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to a partially unsaturated profile, the position of the wetting front can be seen to progress in a predictable fashion through the unsaturated zone. Further work remains to be done comparing the solutions from our simple test problems simulating the movement of the wetting front to available analytical solutions. Test cases also demonstrate both that soil moisture deficits in the unsaturated zone are met before the saturated zone begins receiving recharge and evapotranspiration needs are met from soil moisture before using groundwater. Tests run using this code and larger models (not presented here) indicate that the time necessary to run this module is not prohibitive. Further planned refinements to the module include simulation of the root zone evapotranspiration more explicitly through the use of more information about the type of vegetation present in the model area and the simulation of the changing ability of roots to extract moisture with increasing depth.

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Errata
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There are errors in two of the equations presented in the paper. These errors are only typographic. The code described in the paper is consistent with the corrected equations.

Equation 1b should read:

Van Genuchten Equation to calculate total head [Equation 1b]

$$h = -\frac{1}{\alpha}\left[\frac{1}{SE^{1/m}} - 1\right]^{1/n} + z$$

where h = total hydraulic head, α = constant, SE = effective saturation, m = constant, n = constant, and z = elevation head

Equation 2 should read:

Van Genuchten approximation of relative hydraulic conductivity [Equation 2]

$$\frac{K(\theta)}{K_{sat}} = \left(\frac{\theta - \theta_r}{\phi - \theta_r}\right)^{1/2}\left[1 - \left(1 - \left(\frac{\theta - \theta_r}{\phi - \theta_r}\right)^{1/m}\right)^{m}\right]^{2}$$

where $K(\theta)$ = relative hydraulic conductivity,
K_{sat} = saturated hydraulic conductivity,
θ = water content, θ_r = residual water content,
ϕ = porosity, α = constant, n = constant, m = constant