ground water
Software Spotlight/ Motomu Ibaraki, Software Editor

MODFLOW-NWT: Robust Handling of Dry Cells Using a Newton Formulation of MODFLOW-2005

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Introduction

The first versions of the widely used groundwater flow model MODFLOW (McDonald and Harbaugh 1988) had a sure but inflexible way of handling unconfined finite-difference aquifer cells where the water table dropped below the bottom of the cell—these "dry cells" were turned inactive for the remainder of the simulation. Problems with this formulation were easily seen, including the potential for inadvertent loss of simulated recharge in the model (Doherty 2001; Painter et al. 2008), and rippling of dry cells through the solution that unacceptably changed the groundwater flow system (Juckem et al. 2006). Moreover, solving problems of the natural world often required the ability to reactivate dry cells when the water table rose above the cell bottom. This seemingly simple desire resulted in a two-decade attempt to include the simulation flexibility while avoiding numerical instability.

Early attempts at "re-wetting" dry cells in MODFLOW, such as BCF2 (McDonald et al. 1992) were found to work for some, but not all, MODFLOW models. Re-wetting of dry cells was often numerically unstable and prevented model convergence (Doherty 2001; Painter et al. 2008). When BCF2 did have a stable solution, the resulting runtimes were appreciably longer, the effort to select suitable BCF2 settings was often large, and the solution did not robustly handle input perturbations of parameter estimation (Doherty 2001). Moreover, BCF2 settings that worked in one model did not necessarily translate well to another. Various "home-brewed" alternative versions of MODFLOW were also developed during this time that added a small amount of water to each dry cell after each iteration thereby leaving each cell with a small but non-zero transmissivity, the most popular and full-featured being that of Doherty (2001). However, even model stability using this formulation was found to rely on less-than-intuitive parameter settings that required effort to customize. Moreover, there were still large numbers of groundwater flow problems that remained unstable even with this modification (Doherty, written communication, 2012). Thus, even though some proprietary versions of MODFLOW had better handling of dry cells, many modelers substituted shortcuts within MODFLOW; shortcuts such as assuming all layers were confined, artificially lowering cell bottoms, and large convergence criteria—non-physical adjustments that "could raise questions about the accuracy and reliability of the model results" (Painter et al. 2008).

After two decades of work, the general solution scheme used in MODFLOW was still simply not capable of robustly handling wet-dry problems, especially where the number of dry cells was non-negligible (Painter et al. 2008). This realization led to a new approach to solving the equations used by MODFLOW, one using a Newton-Raphson solution rather than a Picard method—see Mehl (2006), Painter et al. (2008), Keating and Zyvoloski (2009), and Bedekar et al. (2011) for a more complete description of solution techniques. In our 25 years of experience using MODFLOW, the Newton-Raphson formulation may be the single most important advancement to widely used finite-difference techniques since the release of the original MODFLOW. Version 1.0.5 of MODFLOW-NWT, the three-dimensional Newton-Raphson finite-difference formulation of Niswonger et al. (2011), is the subject of this review.

Overview of Features and Input Required

Although MODFLOW-NWT is an important algorithmic reformulation of the MODFLOW family of

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(Picard-only solver) codes, the application of the updated code is almost entirely transparent to the user. MODFLOW-NWT Packages have the same format as standard MODFLOW-2005 (Harbaugh 2005), with a few notable exceptions.

First, the list of possible Newton-Raphson solver input variables is more extensive than most MODFLOW solvers. Depending on the model application, the NWT solver input file can have over 20 variables specified. In recognition that greater input complexity can hamper efficient use of the solver, MODFLOW-NWT provides keyword alternatives in lieu of specifying each solver variable individually. For example, the user can simply specify the type of problem they are solving, ranging from nearly linear or "simple" "moderate," to highly nonlinear or "complex." MODFLOW-NWT is well suited for highly nonlinear problems, such as those with nonlinear stress packages (e.g., Multi-Node Well Package), and/or one or more unconfined layers representing complex geology and groundwater-surface water interaction. In addition to new Newton-Raphson solvers (the χMD and GMRES routines), other familiar MODFLOW-2005 Picard solvers are also available within MODFLOW-NWT.

Secondly, an "upstream weighting" (UPW) Package is used instead of the Layer-Property Flow (LPF) and Block-Centered Flow (BCF) Packages used by MODFLOW-2005. Upstream weighting is an alternative approach for calculating intercell conductance that is analogous to the intercell averaging of relative permeabilities used in unsaturated and multiphase flow codes (Painter and Seth 2003). Painter et al. (2008) describe a simple upstream weighting approach in these terms: if flow is from cell i to cell j, upstream weighting uses hydraulic head in the upgradient cell i to calculate the average saturated thickness and intercell conductance for the pair of cells. In practice this means that upstream weighting restricts flow leaving a cell, which in turn causes the cell to contribute negligible or zero flow and storage when the water level approaches or falls below the cell bottom elevation (Figure 1a and 1b). The UPW Package smoothes the horizontal-conductance function and the storage-change function during wetting and drying of a cell to provide continuous derivatives for solution by the Newton method (Niswonger et al. 2011). The smoothness of the transition allows a cell to remain active even when it has completely dewatered, thus helping to avoid numerical instabilities described previously. Instead of converting abruptly to 0 as the unconfined cell dries, conductance and storage values approach 0 along a gradual slope at small saturated thicknesses (Figure 2a).

This formulation addresses the potential for unrealistic loss of recharge that can occur with dry cells noted previously. If a cell is dry (that is, head is below the cell bottom) and underlain by a fully or partially saturated cell, its horizontal conductance will be 0 and the head in the dry cell can be calculated in terms of the sum of inflow to the cell from adjacent cells and from external sources (Figure 1b). The head calculated for the dry cell is the head that provides an outflow rate that is equal to the inflow rate to the cell (thus insuring mass balance), but it is not the altitude of the water table (Niswonger et al. 2011) which, instead, corresponds to the head in the topmost cell at the row/column location which is at least partially saturated.

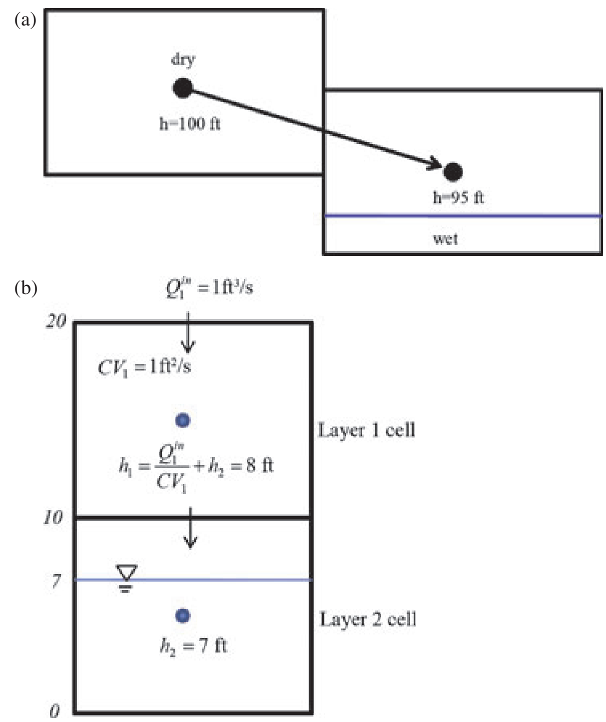

Figure 1. (a) Water flowing out of an active yet dry cell. MODFLOW-NWT eliminates this flow by setting the conductance between the two cells equal to 0. (b) A two-layer model in which recharge is applied to layer 1 (cell 1) and the water table is in layer 2 (cell 2). Layer 1 is dewatered and has a head below the bottom of layer 1 (source Niswonger et al. 2011).

Although this useful formulation is different from the LPF Package, MODFLOW users familiar with the LPF Package will have no trouble recognizing the input variables and formats associated with the UPW Package required by MODFLOW-NWT—UPW is almost identical to the LPF Package! From a functionality view, UPW differs from LPF in that it only supports a single formulation for calculating vertical conductance, calculated as the conductance of two one-half cells in a series with continuous saturation between them (Harbaugh 2005, 5–8). Optional interpretations of the groundwater storage input variable are also not supported by the UPW Package. Consequently, the MODFLOW-2005 LPF Package input variable "OPTIONS" is not supported by the UPW Package. Most importantly, unlike the LPF Package, in which cells will be removed from the simulation if the head is below the cell bottom, MODFLOW-NWT will not set a dewatered cell to no flow. Therefore no rewetting information is needed, or allowed, in the UPW Package input file. All initially active cells remain active even if dry.

Finally, although the Well (WEL) Package for MODFLOW-2005 can be used directly by MODFLOW-NWT, there is an additional option designed to facilitate

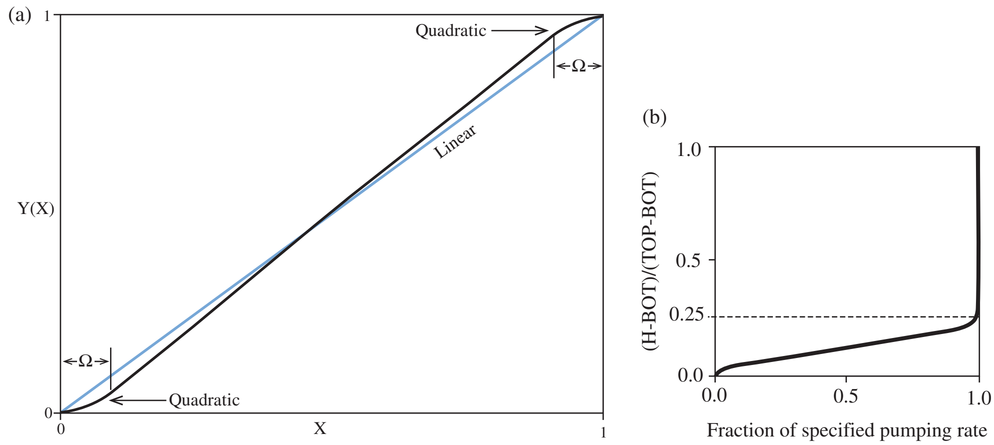

Figure 2. (a) Linear and quadratic functions used to smooth conductance and storage in MODFLOW-NWT (black) compared to linear function that is used by MODFLOW-2005 (blue). *X* is the saturated thickness divided by the cell thickness, *Y* is the value of the smoothing function, and Ω is the interval of *X* where the quadratic equation is applied (source Niswonger et al. 2011). Ω is a solution input variable set to 0.1 in this example, but typically set several orders of magnitude smaller than 0.1 in model applications. (b) Curve used to smoothly reduce specified pumping to 0 when cell dewaters; the MODFLOW-NWT variable PHIRAMP (symbolized as Φ by Niswonger et al. 2011) is the saturated thickness in an unconfined cell at which pumping begins to be reduced, In this example it is set to 0.25. The default value for Φ is 0.05, but the user can select smaller or larger values to test the effect on the pumping rate sustained by the simulation when partial dewatering of the cell occurs.

pumping in thin unconfined layers (Niswonger et al. 2011). A smoothing function similar to that for conductance and storage is enforced for pumping (Figure 2b) such that the discharge rate does not change abruptly to 0 when the head falls below the unconfined cell bottom. Rather, the rate is adjusted based on the simulated saturated thickness. The user-specified variable for the saturated thickness threshold below which pumping decreases (called PHIRAMP) can range between 0.0 and 1.0. The default setting of 0.05 can be overridden in the WEL package. For unconfined cells, well pumping is limited by the amount of water in the cell; any instances of reduced pumping rates due to loss of saturated thickness below the PHIRAMP threshold are reported in the Listing File (Figure 3) or to a separate output file. In this way MODFLOW-NWT simulates the pumping that can be sustained by a well given the values selected for input parameters such as transmissivity and recharge. Information on sustainable pumping rates often has an analogue in the field, making this type of model output ideal for helping to constrain parameter estimates during the calibration process.

Advantages and Disadvantages

Simply put, MODFLOW-NWT can transform the modeling experience. Modelers no longer need expend time and effort fighting solution instability resulting from dry nodes, or be forced to address initial head sensitivity while making subjective judgments of what constitutes an acceptable dry cell distribution for a site area. Instead, modelers can focus on fitting the numerical model to the conceptual model and observed field data. For example, in a watershed setting similar to that found to be problematic by Juckem et al. (2006), a coupled groundwater-surface water model (GSFLOW—Markstrom et al. 2008) using MODFLOW-2005 had over 1400 timesteps of a 8400 timestep simulation period characterized by non-conver gence when solved using the Preconditioned Conjugate-Gradient solver (PCG2—Hill 1990). When the same coupled groundwater-surface water model was run with MODFLOW-NWT substituted for MODFLOW-2005, every timestep of the simulation period converged, with no appreciable increase in the model run time (R.J. Hunt, U.S. Geological Survey, unpublished data).

In another case that featured fine grid spacing and thin layers to properly simulate diversion of water from streams to riverbank wells (Feinstein et al. 2012), initial model runs with the PCG2 solver did not achieve a stable solution due to thousands of locations where active wet cells in layer 1 overlay inactive dry cells in deeper layers (Figure 4a). The layer 1 cells would, in many cases, be isolated from surrounding cells (the intercell

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WELLS WITH REDUCED PUMPING FOR STRESS PERIOD     1 TIME STEP     1
   LAY    ROW    COL          APPL.Q           ACT.Q          GW-HEAD         CELL-BOT
     4      1    175   -0.105500E+01  -0.746625E+00    0.958788E+03    0.952360E+03
     1      1    407   -0.237950E+01   0.000000E+00    0.849039E+03    0.857060E+03
     1      1    412   -0.820176E+02  -0.249923E+02    0.857447E+03    0.855980E+03
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Figure 3. Sample output from MODFLOW-NWT listing file (Feinstein et al. 2012) showing the reduced pumping rate sustained by the simulation along with saturated thickness information at several partly dewatered cells containing wells. In this case Φ was set to 0.2.

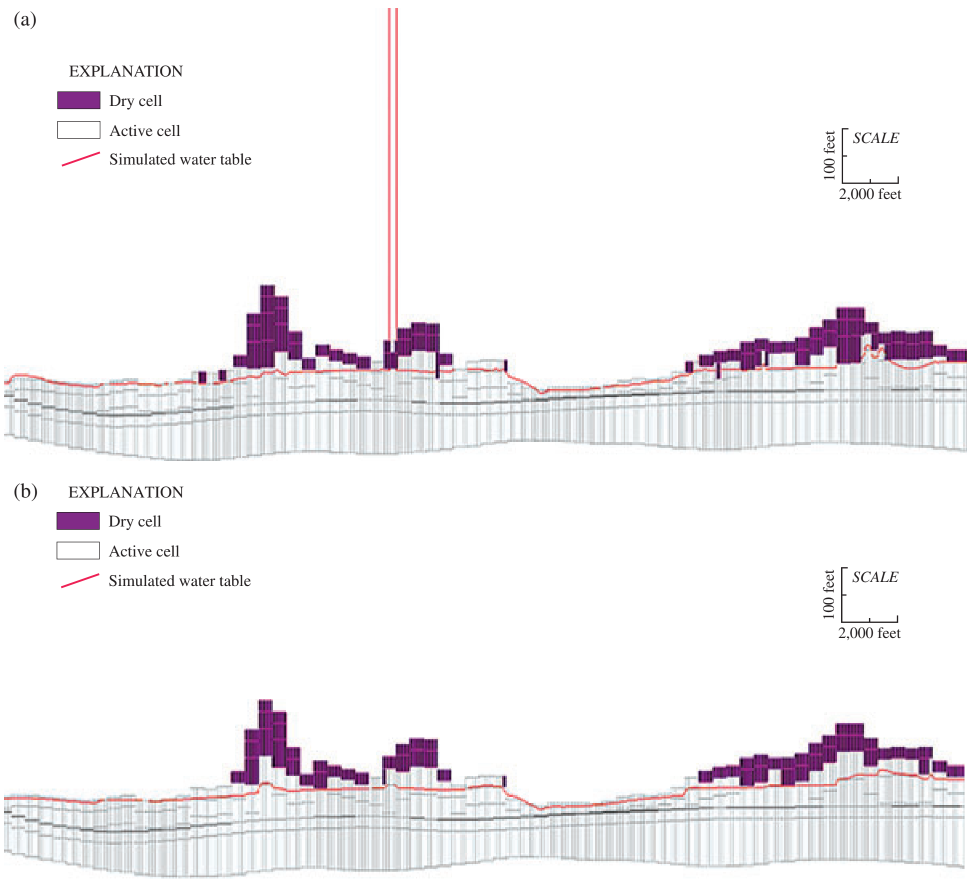

Figure 4. Water table solution along sample row of model using: (a) MODFLOW-2005 with PCG2 solver; and (b) MODFLOW-NWT with χMD solver. (Feinstein et al. 2012). PCG2 yields a perverse water table solution due to the presence of an active cell over an inactive dry cell. χMD yields a smooth solution because the dry cells remain active.

conductance having fallen to 0), and the recharge applied to the shallow active cells would accumulate, yielding unacceptably high water table elevations. This type of problem is not uncommon in MODFLOW models that target groundwater/surface-water interactions and use thin upper layers. Substituting the NWT-χMD solver for PCG2 completely eliminated the confounding artifact, produced a smooth water table solution (Figure 4b), and allowed the model to be calibrated and applied to a range of management scenarios.

The MODFLOW-NWT documentation is extensive and gives in-depth coverage of the theory and implementation of under-the-hood changes. However, the documentation focuses on differences with respect to the widely used MODFLOW-2005 model of Harbaugh (2005); thus a user will have to be familiar with MODFLOW-2005 to fully access all packages available in MODFLOW-NWT. Because MODFLOW-NWT is so similar to MODFLOW-2005, it can be easily integrated into the existing suite of MODFLOW graphical user interfaces (GUIs), and some GUIs have already added MODFLOW-NWT to their latest releases.

One potential issue for MODFLOW-NWT is that the new solver variables and associated documentation are more extensive (and complex) than existing MODFLOW Picard solvers. General guidelines for selection of optimal input for the Newton-Raphson solver are not fully developed. Moreover, changes to solver parameters can have large effects on model run times. As a result, initial use of MODFLOW-NWT will require a high degree of model input and output evaluation by the user to ensure that this new and powerful reformulation of MODFLOW is running at full speed.

Summary

MODFLOW-NWT provides easy access to robust handling of dry cells previously unavailable to a generation of MODFLOW modelers. It is a powerful, sophisticated, and open-source/free resource for both researchers and practitioners, which is already being incorporated in graphical user interfaces. Given our positive experience with MODFLOW-NWT in traditionally difficult settings, we believe it is well-suited to become a standard tool in the hydrogeologist's modeling toolbox.

How to Obtain the Code and Documentation

MODFLOW-NWT and related documentation are available to public from the U.S. Geological Survey free of charge. They can be downloaded from: http://water.usgs.gov/nrp/gwsoftware/modflow_nwt/ModflowNwt.html.

Reviewers

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