Final Technical Report for

ROBUST REPRESENTATION OF DRY CELLS IN MODFLOW

SwRI Project 20-13003

Prepared for

Edwards Aquifer Authority
1615 N. St. Mary's Street
San Antonio, TX 78215

May 2007

SOUTHWEST RESEARCH INSTITUTE®
SAN ANTONIO, TEXAS
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QUALITY ASSURANCE STATEMENT

No GED-generated original data are contained in this report. The analyses contained in this report are documented according to GED quality assurance procedures in Scientific Notebooks SN871E and SN854E. MODFLOW-NR was developed using GED quality assurance procedure TOP-018.

INTRODUCTION

The Edwards Aquifer Groundwater Management Model (EAGWMM) [Lindgren et al., 2004] is based on the industry-standard MODFLOW [Harbaugh et al., 2000] groundwater modeling system. When MODFLOW calculates a water level that is below the base elevation of a computational cell, that cell is declared to be dry and removed (temporarily or permanently) from the calculation. This dry-cell handling algorithm may prevent the MODFLOW outer iteration scheme from converging [MacDonald et al., 1992]. Moreover, if the dry cell has a specified recharge or pumping rate, then making it inactive causes a non-physical change in the global water balance. These problems with the MODFLOW system are well-known and long-standing. Recent experience [Beech, 2006] with the EAGWMM indicates that the dry-cell issue is a significant obstacle to practical applications. Although previous attempts to correct the problem have been published [Doherty, 2001; HydroGeoLogic, 2006], these have met with only limited success.

This report describes a new variant of MODFLOW, denoted MODFLOW-NR, that incorporates a recently developed robust computational scheme [Painter et al., 2007] for representing dry cells. The new representation of dry cells, which was originally developed for the Edwards Aquifer Authority (EAA) and Southwest Florida Water Management District as part of a karst modeling project [Painter et al., 2007], combines an upstream-weighting algorithm for intercell conductances with a new solver package. This report summarizes the capabilities, technical basis, data input requirements, software validation/verification tests, and example simulations for the MODFLOW-NR software.

OVERVIEW OF MODFLOW-NR

MODFLOW-NR is a non-standard variant of MODFLOW that was derived from MODFLOW-2000 Version 1.12.01. The modifications of MODFLOW-2000 that resulted in MODFLOW-NR include the addition of a new groundwater flow package denoted Upstream Weighted Flow (UWF), the addition of a new solver package (denoted NR1) based on the Newton-Raphson method, and minor modifications to the main program and the Well and Horizontal Flow Barrier (HFB) packages. The improved representation of dry cells resulted in a MODFLOW variant, not a self-contained MODFLOW package, because the NR1 solver requires data exchange that is not compatible with the standard MODFLOW data structure. MODFLOW-NR Version 1.0 is limited to single-layer aquifers.

The UWF package is the only groundwater flow package option in MODFLOW-NR. The UWF package is based on the Layer Property Format (LPF) package and takes input that is identical to the input required by the LPF package.

The NR1 solver is the only solver option available in MODFLOW-NR. NR1 uses the Newton-Raphson method for the MODFLOW outer iteration process that is used to resolve nonlinearities in MODFLOW. All publicly available (noncommercial) versions of MODFLOW use a simple variable substitution (Picard) iteration scheme. The Newton-

Raphson method has long been understood to be more robust and computationally efficient, but is more difficult to implement than the Picard scheme.

The modifications to the Well and HFB packages were relatively minor. The HFB package was modified to provide information needed by the NR1 solver. The Well package was modified to ramp down the pumping rate when the water level approaches the bottom elevation of a cell. The input formats and requirements for the modified Well and HFB packages are identical to the standard Well and HFB packages.

DRY CELL REPRESENTATION IN MODFLOW-NR

In MODFLOW-NR, hydraulic head in a cell is never allowed to drop below the bottom elevation of that cell. If an outer iteration calculates a hydraulic head that is below the bottom elevation of a cell, the updated head for that cell is set equal to the arithmetic average of the previous head and the cell bottom elevation. This procedure allows the head in a cell to become arbitrarily close to the cell bottom over the course of several iterations. However, the head will always be greater than the cell bottom, thus allowing the cell to remain active in the calculation and avoiding unwanted changes to the global water balance.

To work properly, the updating scheme just described must be combined with an upstream weighting for the intercell conductances (branch conductances in MODFLOW terminology). Upstream weighting refers to an averaging process used to calculate intercell conductances from hydraulic head values in neighboring cells. If flow is from cell *i* to cell *j*, upstream weighting uses hydraulic head in cell *i* to calculate saturated thickness and intercell conductance for the pair of cells. This is in contrast to the conventional MODFLOW approach, which uses a symmetrical averaging (e.g. arithmetic) of the two hydraulic heads. Upstream weighting is widely used in unsaturated and multiphase subsurface flow codes. The principal advantage of upstream weighting is that it prevents flow from leaving a nearly dry cell while allowing flow to return to a nearly dry cell if any of the neighboring heads are higher than the cell in question.

To express the upstream weighting in a compact form, a simplified, albeit non-standard, notation is useful. Let h_{j+} denote the hydraulic head in upstream cell $j+1,i,k$, and let h denote the head in cell j,i,k. Similarly, let CR_+ denote the row conductance between cells j,i,k and $j+1,i,k$. In standard MODFLOW notation, that row conductance is denoted $CR_{j+1/2,i,k}$. In the notation used here, the row conductance is then expressed as

$$CR_+ = K_+ \left\{ \min\left(Z_{j+}^{top}, \max\left(h_{j+}, h\right)\right) - Z_{j+}^{bot} \right\} \tag{1}$$

where K_+ is the harmonic averaging of the hydraulic conductivities for cells j,i,k and $j+1,i,k$, and Z_{j+}^{top} and Z_{j+}^{bot} are intercell averages for top and bottom elevations. In order to prevent flow from leaving a dry cell, the following definition for Z_{j+}^{bot} is needed:

$$Z_{j+}^{bot} = \max(Z_{j,i,k}^{bot}, Z_{j+1,i,k}^{bot}) \tag{2}$$

We have more flexibility in the definition of the Z_{j+}^{top} parameter, and the following is used in MODFLOW-NR

$$Z_{j}^{top} = \left(Z_{j,i,k}^{top} + Z_{j,i+1,k}^{top}\right)/2\,. \tag{3}$$

NEWTON-RAPHSON SOLVER

For unconfined aquifers, the groundwater flow equations solved by MODFLOW are nonlinear because the branch conductances depend on saturated thickness and thus the dependent variable (hydraulic head).

The conventional MODFLOW system uses a Picard iteration strategy to resolve the nonlinear terms. With Picard iterations, the branch conductances are calculated using the hydraulic head from the previous iteration. The branch conductances are then held fixed while the head is updated by solving the resulting linear system. This iterative process is repeated until the head changes very little between subsequent iterations. The solution to the linear system itself may also be accomplished by an iterative process. Iterations to solve the linearized system are typically referred to as “inner iterations” and the process of iteratively updating the head and branch conductances as “outer iterations.” All non-proprietary solver packages in the conventional MODFLOW system use a variant on the Picard iteration strategy for the outer iterations.

Picard iteration is generally adequate for mildly nonlinear systems, but may fail to converge or require an excessive number of iterations for more strongly nonlinear systems. The NR1 solver uses the Newton-Raphson method. The Newton-Raphson method for solving nonlinear equations is more robust than the Picard scheme because it uses derivative information in the iterations. The Newton-Raphson method is, however, more difficult to implement than the Picard iteration scheme and requires more information from the groundwater flow packages.

The groundwater flow equation system, discretized with respect to space and time, can be written in symbolic form as

$$\mathbf{R}(\mathbf{h}) = \mathbf{0} \tag{4}$$

where $\mathbf{R}$ is the residual vector representing cell-by-cell errors in water balance and $\mathbf{h}$ is the head vector. An explicit form for the discretized groundwater flow equations is given in the Appendix. Let $\mathbf{h}^m$ and $\mathbf{R}^m$ denote the head approximation and resulting residual vector at iteration *m*. In the Newton-Raphson method, the next iteration of the head is obtained as $\mathbf{h}^{m+1} = \mathbf{h}^m + \mathbf{\Delta}^m$ where $\mathbf{\Delta}^m$ is the solution to the linear system

$$\mathbf{J}^m \mathbf{\Delta}^m = -\mathbf{R}^m \tag{5}$$

Here $\mathbf{J}^m$ is the Jacobian matrix. The entry J_{pq} in the p-th row and q-th column of that matrix is the derivative of the p-th residual with respect to the q-th hydraulic head, $J_{pq} = \dfrac{\partial R_p}{\partial h_q}$. Explicit forms for the Jacobian matrix are given in the Appendix.

The NR1 solver implements a slight variation on the classical Newton-Raphson method by employing an adaptive damping strategy. The adaptive damping algorithm is a modification of Cooley's method [1983]. The algorithm monitors for oscillations in the iteration procedure and applies damping if oscillations are detected.

The linear system given by equation 5 is solved in the NR1 solver by a pre-conditioned conjugate gradient algorithm. Incomplete lower-upper (ILU) decomposition with fixed level of fill is used for the preconditioner. Iteration acceleration is by the biconjugate gradient stabilized (BCGSTAB) method. The algorithms for solving the linear system are described in detail by Saad [2003].

INPUT FORMAT FOR MODFLOW-NR

Name File

MODFLOW-NR requires use of the UWF package, which is activated by adding the following line to a MODFLOW name file

```
UWF   Nunit   Fname
```

where Nunit is the Fortran unit to be used for file I/O and Fname is the name of the I/O file. Note that UWF must be specified.

UWF is designed to work with the new Newton-Raphson solver NR1. The NR1 solver will be activated automatically. Other MODFLOW solvers (i.e., PCG2, GMG, DE4, SIP, etc.) are deactivated if they are included in the name file.

NR1 Solver Input

The NR1 solver input is read from a file called nr1in.dat. The file must be named nr1in.dat. If the file is not present, default values will be used for all input parameters.
The NR1 input is given below.

1. ITMXO HTOL RTOL
2. ATYPE LEVEL NVECTORS DETAIL
3. ITMAXI R2TOL RXTOL SXTOL

Definitions for the input parameters follow.

ITMAX0 – is the maximum number of outer iterations.

HTOL – is the head tolerance [L] used to define convergence in the outer iterations.

RTOL – is the residual tolerance [L^3/T] used to define convergence in the outer iterations.

ATYPE – is an integer-controlling selection of accelerator in a preconditioned conjugate gradient linear solver. Currently, the only allowed value is 4, which corresponds to the bi-conjugate gradient stabilized method. Alternative values may be available in future versions.

LEVEL – is the level of infill allowed in the incomplete lower-upper decomposition used for preconditioning. Recommended values are 1 or 0.

NVECTORS – is read but not currently used.

DETAIL – is an integer controlling output from the linear solver. Enter 0 for no output, 1 for summary output, and 2 for residual information at each inner iteration. Output is written to the file NR1OUT.DAT.

ITMAXI – is the maximum number of inner iterations.

R2TOL – is a convergence criterion for the linear solver based on the Euclidian norm of the residual.

RXTOL – is a convergence criterion for the linear solver based on the maximum residual.

SXTOL – is a convergence criterion for the linear solver based on the maximum scaled solution update.

SOFTWARE VALIDATION TESTS

Numerical tests were used to help ensure that the underlying model equations were correctly implemented in MODFLOW-NR. This process is referred to as “software validation” in this report and should not be confused with model validation/verification, which seeks to build confidence in the underlying models. The underlying model in MODFLOW-NR is the widely accepted Darcy’s law, as in MODFLOW-2000. The software validation strategy is to make direct comparisons between MODFLOW-2000 and MODFLOW-NR for simulations that are not plagued by dry cells.

Validation Test 1

Validation Test 1 uses the two-dimensional configuration shown in Figure 1. All of the boundaries are specified as no-flow. Recharge is specified for approximately 1/3 of the model in the region shown. Discharge is from a spring specified with the MODFLOW Drain Package and by pumping from one well. The spring elevation is 180 m, and the well pumping rate is 0.003 m^3/s. The simulation has a steady-state period and a two-month transient. The specified recharge rate is 0.31 m/yr in the steady-state period and is turned off during the transient period. The bottom of the aquifer is flat with an elevation of 0 m.

Differences in the hydraulic head calculated by MODFLOW-2000 and MODFLOW-NR are to be expected because of differences in the calculation of intercell conductances. Both use harmonic averaging of the hydraulic conductivity. MODFLOW-2000 combines this with an arithmetic average for saturated thickness, whereas MODFLOW-NR uses the upstream-weighting algorithm.

With variations in bottom elevation eliminated, the upstream-weighting algorithm for intercell conductances should give similar results to the conventional MODFLOW-2000 spatial differencing scheme, provided head gradients are not too steep. Thus, this simulation is designed to verify that MODFLOW-NR recovers MODFLOW-2000 results in a situation where the two spatial differencing schemes should produce similar results.

Hydraulic head contours during the steady-state period are shown in Figure 2. The MODFLOW-2000 and MODFLOW-NR contours closely approximate each other. The maximum difference is 0.085% of the total head variation in the simulation. The root-mean-square error is 0.038% of the total head variation.

Hydraulic head contours at the end of the two-month transient period are shown in Figure 3. The maximum difference is 0.089% of the total head variation in the simulation. The root-mean-square difference is 0.040% of the total head variation. This close agreement with MODFLOW-2000 provides confidence that the numerical algorithms used in MODFLOW-NR are correctly implemented.

Validation Test 2

Validation Test 2 uses the same configuration as Validation Test 1, but with a highly variable aquifer bottom (Figure 4). This simulation is designed to provide some insights into consequences of the upstream weighting in the spatial differencing scheme. Larger differences between MODFLOW-2000 and MODFLOW-NR are to be expected with the large variations in aquifer bottom elevation.

Steady-state head contours are compared in Figure 5. The maximum difference in head between MODFLOW-NR and MODFLOW-2000 is 1.1% of the total head drop. The root-mean-square difference is 0.72%.

DEMONSTRATION SIMULATIONS

Two simulations were used to demonstrate the robust functioning of MODFLOW-NR for scenarios of interest. These two simulations represent acceptance tests for the software.

Acceptance Test 1

Acceptance Test 1 is designed to test the robustness of MODFLOW-NR in situations with many dry or nearly dry cells. Test 1 is a one-dimensional simulation of an unconfined aquifer. The head on the right boundary is held constant at 60 m elevation. The left boundary is no-flow. The domain is 1950 m long and divided into 39 cells. A pumping well is located 500 m from the left boundary. Recharge is uniformly distributed along the entire length of the simulation domain. Aquifer top and bottom elevations are shown in Figure 6. The hydraulic conductivity is 2×10^{-5} m/s. The specific storage and specific yield are 10^{-5} and 0.1, respectively.

The simulation has a steady-state period followed by a 12-month transient with one-month time steps. The steady-state period has a specified recharge of 0.31 m/yr and no pumping. The transient period has a pumping rate of 4 m^3/s and no recharge for the first 10 months, followed by a two-month period with a recharge of 1.3 m/yr and no pumping. This scenario is designed to dewater the aquifer and then allow it to recover when recharge returns.

Results in steady state and at several times during the transient simulation are shown in Figure 7; a detailed view from that simulation is shown in Figure 8. This combination of parameters caused many of the cells to approach nearly dry conditions with calculated water levels near the bottom elevations, which is demanding numerically. MODFLOW-NR converged in both steady state and transient conditions without any convergence failures. MODFLOW-2000 was not able to converge for this problem, despite several attempts to adjust the wetting/drying parameters.

Acceptance Test 2

Acceptance Test 2 is the steady-state calibration run plus the first 324 monthly time steps from the transient calibration run of the EAGWMM [Lindgren et al. 2004]. The only adjustments made to the EAGWMM input set were to convert the Block Centered Flow (BCF) input to the LPF input required by the UWF package of MODFLOW-NR, remove some duplicate flow barriers defined in the HFB input, and replace the head initial guess with a constant value.

Steady-state head values are shown in Figure 9. MODFLOW-NR converged to steady state in 20 iterations using an initial guess of 999 for the starting head. Convergence was found to be insensitive to the initial head value, in contrast to the MODFLOW-2000 code, which requires a good estimate of the initial head to converge. MODFLOW-NR's lack of sensitivity to the initial head value is a consequence of the robust handling of dry cells.

MODFLOW-NR completed the 324 monthly steps of the transient calculations without any time step failures. The entire simulation (steady-state followed by 324 transient time steps) required 1 hour 13 minutes on a dual-core 2.2 GHz processor running the Linux operating system.

CONCLUSIONS

The combination of upstream weighting of intercell conductances with a Newton-Raphson solver avoids numerical instabilities and artifacts associated with dry cells. Tests performed to date using the MODFLOW-NR code indicate that the approach is very robust. Comparisons with the unmodified MODFLOW-2000 code demonstrate that the upstream weighting and conventional spatial differencing approaches produce very similar results.

Version 1.0 of MODFLOW-NR is limited to single-layer aquifers. However, the approach is applicable to aquifers with multiple layers. Fully three-dimensional capabilities could be added to future versions with a reasonable level of effort.

MODFLOW-NR has been tested with the Well, Drain, Recharge, River and Horizontal Flow Barrier packages. The recently developed Well Pumping Management Package (WMP1) is not included in Version-1 of MODFLOW-NR, but could be incorporated in future versions.

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APPENDIX

The finite-difference equations for a MODFLOW cell *j,i,k* can be placed in the following form

$$\begin{aligned}&CV_-h_{k-}+CC_-h_{i-}+CR_-h_{j-}+\\&\left(-CV_--CC_--CR_--CR_+-CC_+-CV_++HCOF\right)h+\\&CV_+h_{k+}+CC_+h_{i+}+CR_+h_{j+}-RHS=0\end{aligned} \tag{6}$$

where

$$CV_-\equiv CV_{i,j,k-1/2} \tag{7}$$

$$h_{k-}\equiv h_{i,j,k-1} \tag{8}$$

$$h\ \equiv h_{i,j,k} \tag{9}$$

Other notation is identical to that of the MODFLOW-2000 manual (e.g. Eq 3 of the MODFLOW manual): *CR*, *CC* and *CV* are row, column and vertical conductances, respectively; *HCOF* contains coefficients of head from source and sink terms plus that part of the storage term that multiplies head at the current time level; *RHS* contains constants from source/sink terms plus that part of the storage term coming from the previous time level.

The nonlinear system identified in equation 6 can also be written as

$$\mathbf{R}(\mathbf{h})=\mathbf{0} \tag{10}$$

where $\mathbf{R}$ is the residual vector and $\mathbf{h}$ is the head vector. Let $\mathbf{h}^m$ and $\mathbf{R}^m$ denote the head approximation and resulting residual vector at iteration *m*. The next iteration of the head is obtained as $\mathbf{h}^{m+1}=\mathbf{h}^m+\boldsymbol{\Delta}^m$ where $\boldsymbol{\Delta}^m$ is obtained as the solution to

$$\mathbf{J}^m\boldsymbol{\Delta}^m=-\mathbf{R}^m \tag{11}$$

Here $\mathbf{J}^m$ is the Jacobian matrix with terms defined as $J_{pq}=\dfrac{\partial R_p}{\partial h_q}$.

The diagonal terms of the Jacobian matrix are given by

$$
\begin{aligned}
J_{pp} = {} & \frac{\partial CV_-}{\partial h}\left(h_{k-} - h\right) + \frac{\partial CC_-}{\partial h}\left(h_{i-} - h\right) + \frac{\partial CR_-}{\partial h}\left(h_{j-} - h\right) + \frac{\partial HCOF}{\partial h} h + \\
& \frac{\partial CV_+}{\partial h}\left(h_{k+} - h\right) + \frac{\partial CC_+}{\partial h}\left(h_{i+} - h\right) + \frac{\partial CR_+}{\partial h}\left(h_{j+} - h\right) + D - \frac{\partial RHS}{\partial h}
\end{aligned}
\tag{12}
$$

where

$$
D \equiv \left(-CV_- - CC_- - CR_- - CR_+ - CC_+ - CV_+ + HCOF\right) \tag{13}
$$

and a cell ordering O has been chosen to map the cell coordinates (i,j,k) to position p in the cell list $p = O(i,j,k)$.

Off-diagonal terms are

$$J_{pq} = CV_- + \frac{\partial CV_-}{\partial h_{k-}}\left(h_{k-} - h\right) \quad \text{for } q = O(i,j,k-1)$$

$$J_{pq} = CC_- + \frac{\partial CC_-}{\partial h_{i-}}\left(h_{i-} - h\right) \quad \text{for } q = O(i-1,j,k)$$

$$J_{pq} = CR_- + \frac{\partial CR_-}{\partial h_{j-}}\left(h_{j-} - h\right) \quad \text{for } q = O(i,j-1,k)$$

$$J_{pq} = CR_+ + \frac{\partial CR_+}{\partial h_{j+}}\left(h_{j+} - h\right) \quad \text{for } q = O(i,j+1,k)$$

$$J_{pq} = CC_+ + \frac{\partial CC_+}{\partial h_{i+}}\left(h_{i+} - h\right) \quad \text{for } q = O(i+1,\mathrm{j},k)$$

$$J_{pq} = CV_+ + \frac{\partial CV_+}{\partial h_{k+}}\left(h_{k+} - h\right) \quad \text{for } q = O(i,j,k+1).$$

It is clear from this that six new arrays are required in addition to those already assembled in the MODFLOW system:

$$DCRM = \frac{\partial CR_+}{\partial h} \qquad DCCM = \frac{\partial CC_+}{\partial h} \qquad DCVM = \frac{\partial CV_+}{\partial h}$$

$$DCRP = \frac{\partial CR_+}{\partial h_{j+}} \qquad DCCP = \frac{\partial CC_+}{\partial h_{j+}} \qquad DCVP = \frac{\partial CV_+}{\partial h_{k+}}$$

The first three arrays represent the derivative of the branch conductance with respect to the preceding node and the last three arrays represent the derivative with respect to the following node.

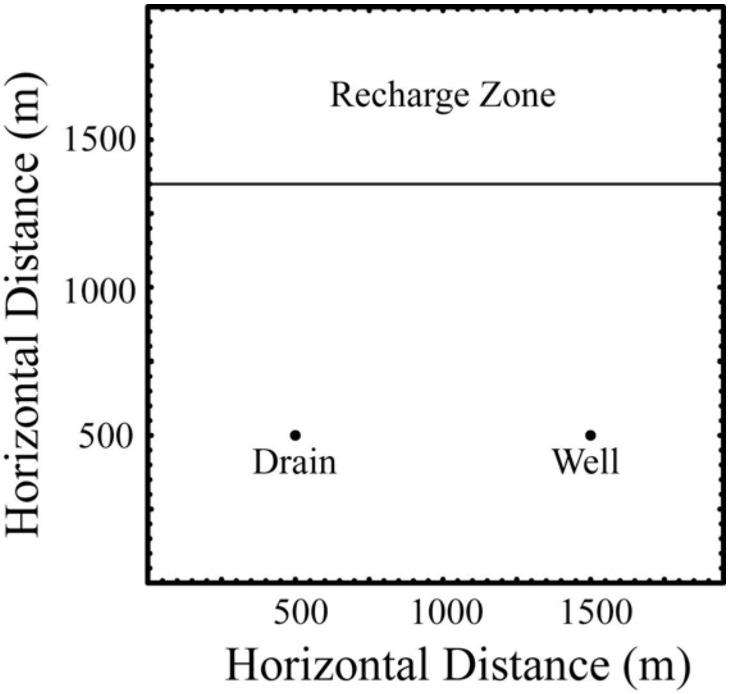

Figure 1. Model domain for validation tests. All boundaries are no-flow boundaries.

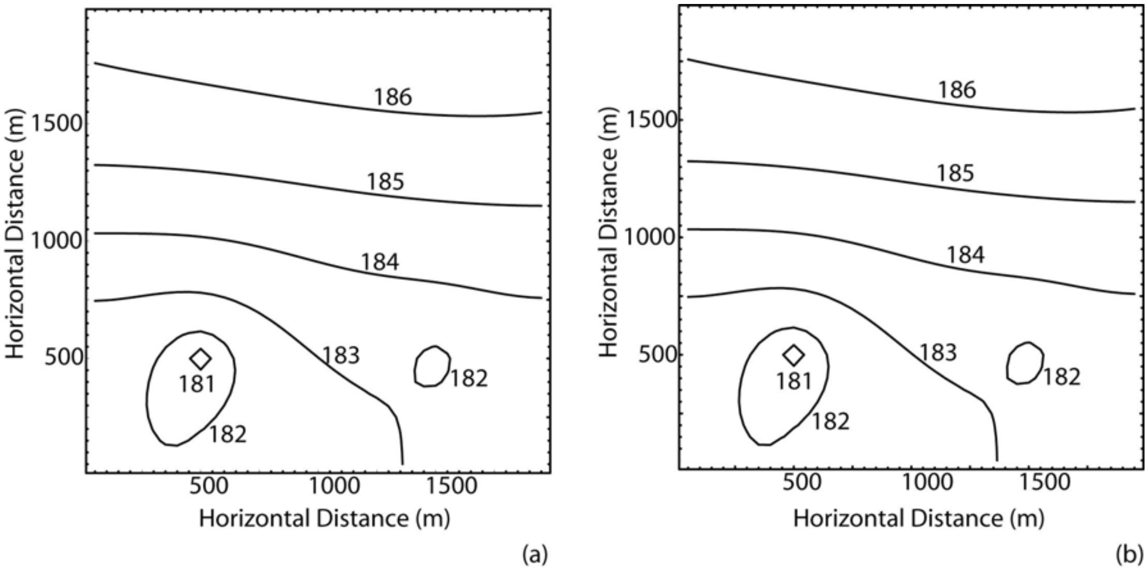

Figure 2. Steady-state hydraulic head contours for Validation Test 1 as calculated by (a) MODFLOW-2000 and (b) MODFLOW-NR.

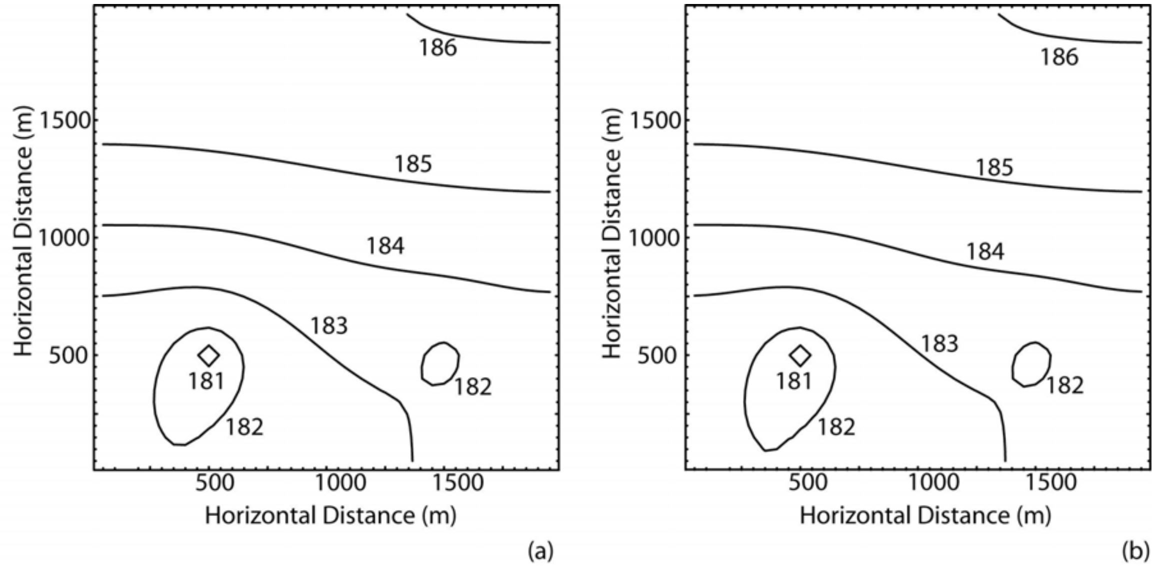

Figure 3. Hydraulic head contours after a 2-month transient for Validation Test 1 as calculated by (a) MODFLOW-2000 and (b) MODFLOW-NR.

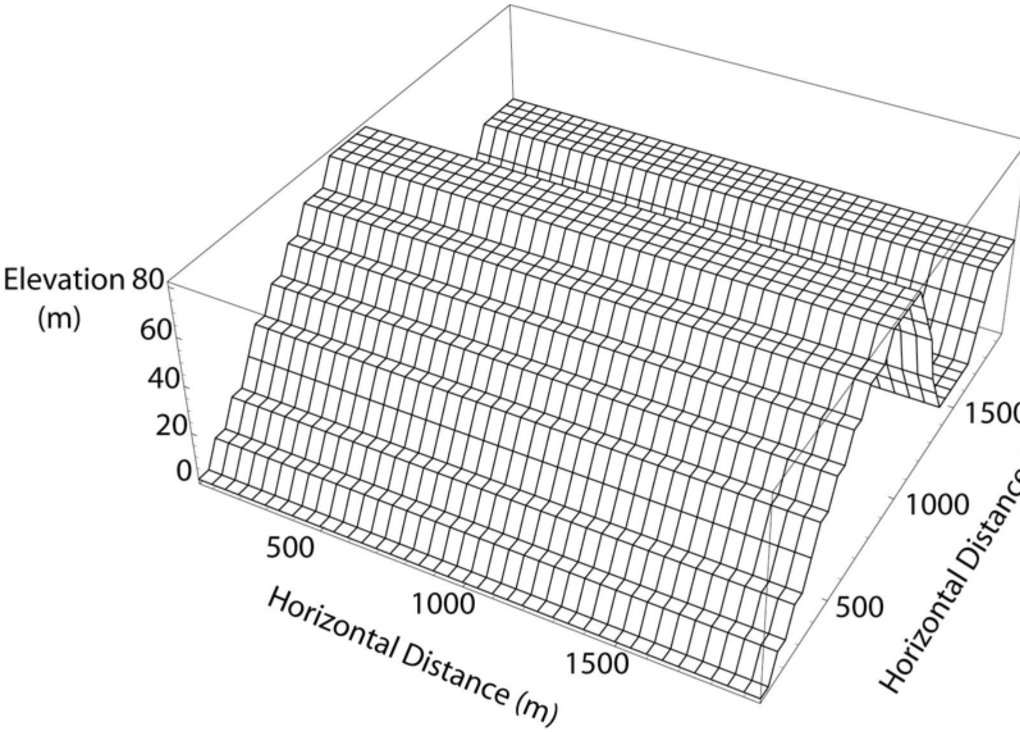

Figure 4. Bottom elevation for Validation Test 2.

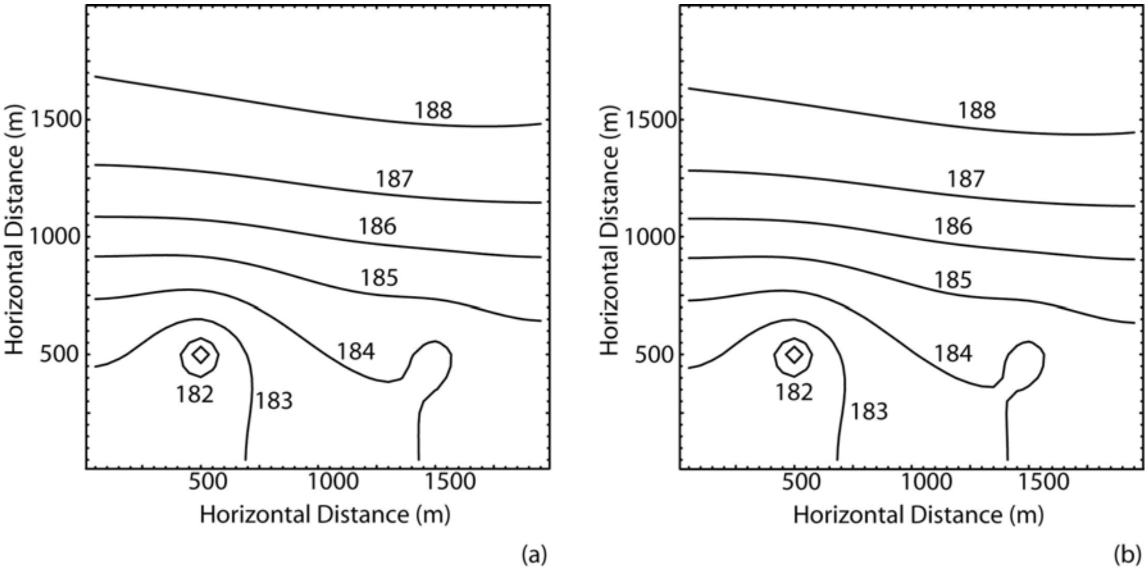

Figure 5. Steady-state hydraulic head contours for Validation Test 2 as calculated by (a) MODFLOW-2000 and (b) MODFLOW-NR.

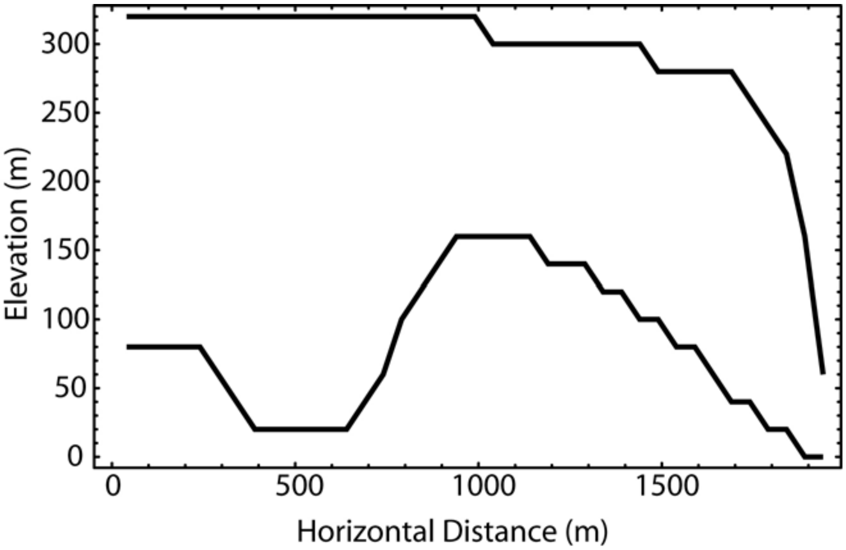

Figure 6. Top and bottom elevations for Acceptance Test 1. In this test, a pumping well is located 500 meters from the left boundary. The right boundary is constant head and the left boundary is specified as no-flow.

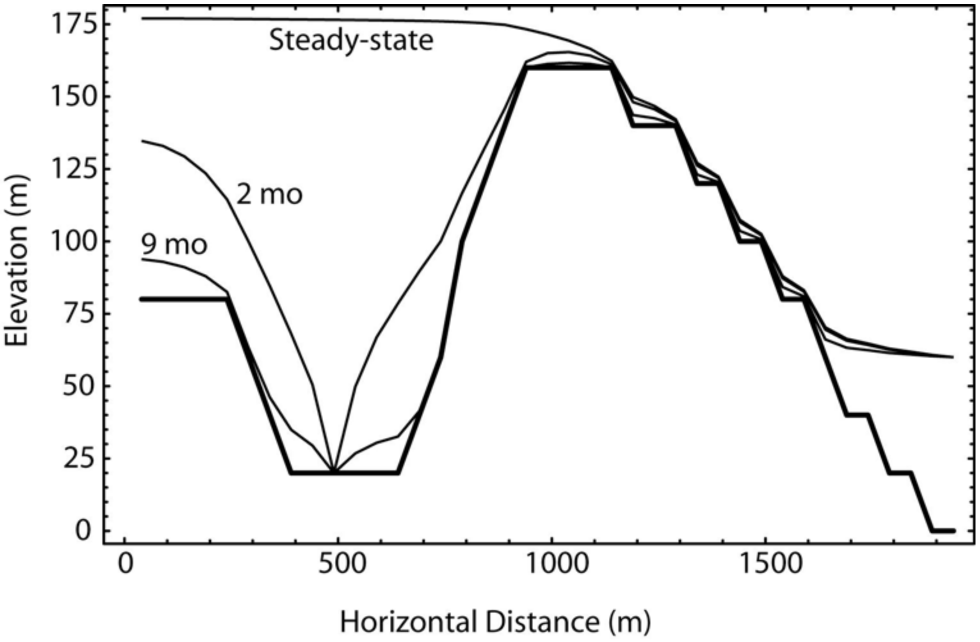

Figure 7. Water level elevations from Acceptance Test 1 for MODFLOW-NR. The bottom elevation is shown as a heavy line.

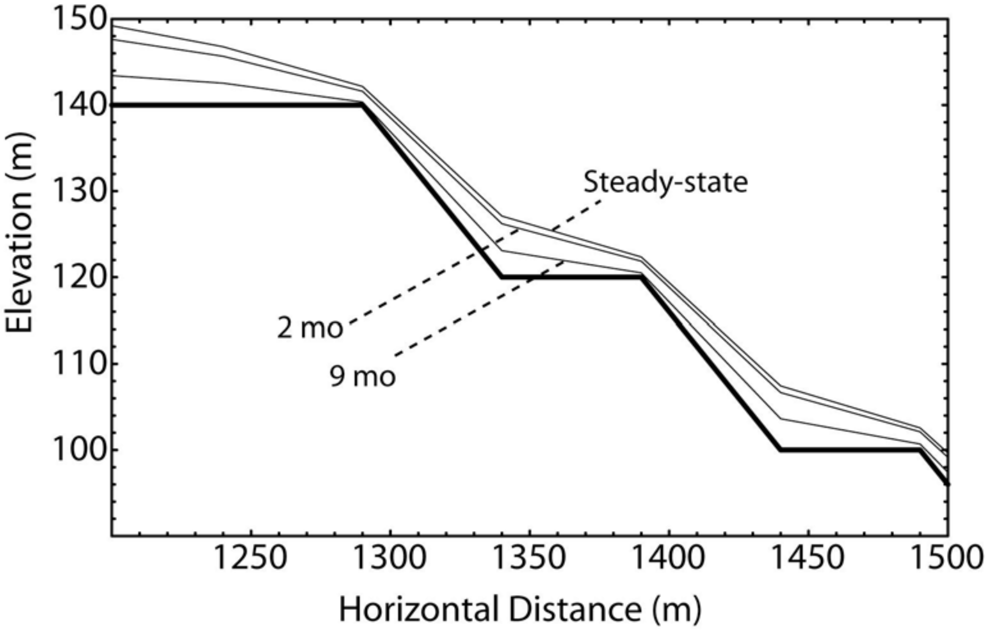

Figure 8. Detail from Figure 7. The bottom elevation is shown as a heavy line.

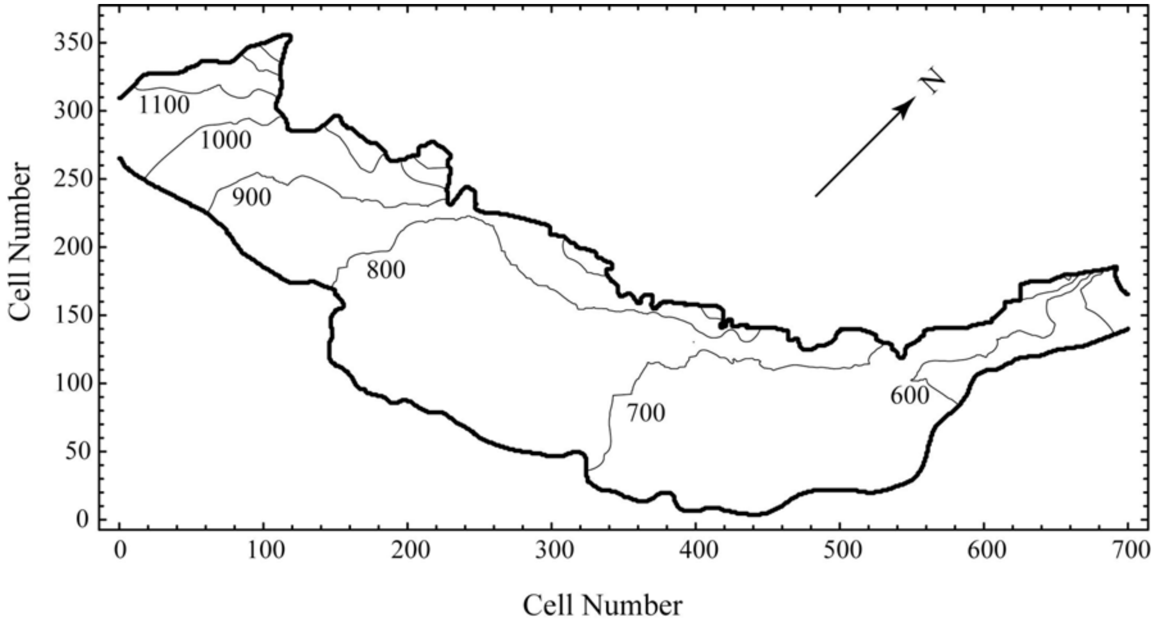

Figure 9. Steady-state hydraulic head contours in feet calculated by MODFLOW-NR using the EAGWMM input. The cells have dimensions 1/4 mi by 1/4 mi (402.3 m by 402.3 m).