Research Paper/

Estimation of the water table position in unconfined aquifers with MODFLOW 6

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Abstract

The numerical estimation of the position of the water table in unconfined aquifers is important for many practical applications. Its determination through observations or analytical methods is restricted to a few cases. Therefore, it is often estimated through numerical simulations, which may be affected by numerical artifacts and/or poor stability.

We use MODFLOW to estimate the position of the water table for a seemingly simple example problem and demonstrate difficulties that can be faced when performing this kind of numerical simulation. We explain the causes for the numerical challenges that originate from the properties of the mathematical equations that must be solved. Based on the results of more than 600 steady-state simulations, we show how the stability of the numerical solution can be affected by the values of physical parameters that define the problem (e.g. recharge rate, anisotropy ratio, and other parameters that control the numerical algorithm such as settings of the linear and non-linear solution methods). Finally, we comment on some best practices to apply numerical simulations to estimate the water table position.

Introduction

The estimation of the water table position in unconfined aquifers is important for assessing groundwater storage, estimating effective recharge and evaluating aquifer vulnerability to downward infiltration from the land surface (Scanlon et al., 2002; Sanford, 2002; Sousa et al., 2013). The determination of the water table position using observed data is difficult due to the need for a dense network of observation points, hence mathematical methods, analytical or numerical, are often used for this purpose (Haitjema, 2006; Bedekar et al., 2012). Analytical solutions based on simplifying assumptions such as homogeneity and hydrostatic pressure distribution are applicable in some cases (Haitjema and Mitchel-Bruker, 2005). However, numerical methods are used in most applications due to their flexibility to model general conditions such as heterogeneous sediments, time variable boundary conditions and spatially variable recharge rates. The exact determination of the water table position through numerical methods requires simulating unsaturated flow, which is still computationally intensive for large-scale models and also prone to numerical stability issues (Farthing and Ogden, 2017).

MODFLOW is a widely used numerical simulator to model groundwater systems (Hughes et al., 2017). It considers three-dimensional groundwater flow in fully saturated porous media. Unless a specialized unsaturated zone flow package or a custom MODFLOW version is used, the underlying MODFLOW equations do not describe three-dimensional (3D) unsaturated flow that takes place within partially saturated materials located between the ground surface and the water table (Langevin et al., 2017). The determination of the water table position with MODFLOW requires solving a partial differential equation (PDE) that is known to be challenging due to the non-linear behavior of the solution and difficulties that arise due to computing the upper boundary of the saturated porous media (water table) using fixed numerical grids (Niswonger et al., 2011).

The numerical solution of the non-linear PDE that represents fully saturated groundwater flow is implemented based on a linearization of the original equation using an iterative Picard or Newton scheme (Langevin, 2017). The iterative algorithms are prone to numerical instabilities because of the discontinuous transition between wet (saturated) and dry (unsaturated) grid cells. Such discontinuities often result in oscillatory numerical approximations that do not converge to a single correct solution. The lack of robust algorithms and solutions to determine the water table position has long been recognized as a main limitation for using MODFLOW to simulate unconfined aquifers (Painter et al., 2008; Bedekar et al., 2012; Hunt and Feinstein, 2012), which can be particularly problematic when the numerical solution is used as part of parameter estimation or uncertainty analysis (Doherty, 2001). Therefore, different approaches have been proposed and implemented in MODFLOW to alleviate such numerical artifacts.

MODFLOW 6 is the current version of MODFLOW distributed by the U.S. Geological Survey (Hughes et al., 2017; Langevin et al. 2017). MODFLOW 6 implements traditional cell wetting and drying methods for water table simulations as well as a non-linear Newton based algorithm, which is based on the approaches developed by Painter et al. (2008), Niswonger et al. (2011), and Panday et al. (2013).

The estimation of the water table position through numerical solutions is further complicated by the large number of options and parameter values that control the numerical solution. Amongst others, the numerical solution depends on the grid cell size or spatial resolution and the parameters that control the level of accuracy of linear and non-linear solvers, e.g. the tolerance value set to evaluate convergence of the iterative linear solvers (Hughes et al, 2017). In the case of MODFLOW 6, there are more than 10 options or parameters to control the non-linear and linear solvers (see Supporting Information for a few examples). Optimal parameter values that ensure fast and reliable convergence of the solution are, in most cases, problem dependent, though some advances have been made in optimizing them (Newcomer and Hunt, 2022). Therefore, the selection of solver parameter values often requires trial-and-error, which makes the estimation of the water table through numerical simulations more problematic and less reliable.

The purpose of this technical article is to demonstrate through an example, the main difficulties that can arise when applying MODFLOW-based programs to determine the position of the water table in unconfined aquifers. We also include a brief summary of the theoretical background that is required to understand those challenges and provide experience-based guidance on how to achieve sensible numerical results for these kinds of applications.

Mathematical Formulation

Mass balance equation

The flow field in fully saturated porous media is modeled by the following equation (Bear, 2012; Langevin et al., 2017),

$$S_S \frac{\partial h}{\partial t} = \nabla \cdot (K \nabla h) + \hat{Q}_s \quad (1)$$

where S_S [1/L] is specific storage, K [L/T] is the hydraulic conductivity tensor, h [L] is the hydraulic head measured with respect to some datum and $\hat{Q}_s$ [1/T] represents sources or sinks. In general, K is a full second order symmetric tensor with six unique components: three diagonal and three off-diagonal coefficients (Provost et al, 2017). However, for most applications, it is assumed that its principal axes coincide with the axes of the coordinate system, so it is reduced to only the diagonal elements K_{xx}, K_{yy} and K_{zz}. In that case, the relative magnitude of the vertical and horizontal flow components depends on the hydraulic gradient, ∇h, and the ratio (anisotropy) of the vertical and horizontal hydraulic conductivity, $\alpha_{vh} = K_v/K_h$.

In groundwater hydrology, it is customary to integrate the previous equation assuming that there is no resistance to vertical flow between an upper (η) and a lower (ξ) elevation, so that the flow can be represented by the following two-dimensional (2D) equation,

$$S\frac{\partial h}{\partial t} = \nabla\cdot\left((\eta - \xi)K_2\nabla h\right) + Q_s \qquad (2)$$

where S [-] is the storage coefficient, K_2 [L/T] includes the components of the hydraulic conductivity tensor in the horizontal direction, and Q_s [L/T] represents the integral of the sources or sinks. We drop the subindex 2 to simplify the notation. The term $(\eta - \xi)$ corresponds to the saturated thickness, so that $T = (\eta - \xi)K$ is the transmissivity of the aquifer section. For unconfined aquifers, the top elevation corresponds to the hydraulic head, $\eta = h$, and the storage coefficient can be written as a combination of the specific storage S_s [1/L] and the specific yield S_y [-] to obtain the following non-linear PDE

$$\left(S_y + S_s(h - \xi)\right)\frac{\partial h}{\partial t} = \nabla\cdot((h - \xi)K\nabla h) + Q_s \qquad (3)$$

Dupuit approximation

Considering a 2D cross-section that receives a constant recharge rate R [L/T] as shown in Figure 1, and assuming steady-state conditions, negligible vertical gradients and $\xi = 0$, equation (3) becomes

$$- \frac{\partial}{\partial x}\left(hK \frac{\partial h}{\partial x}\right) = R \qquad (4)$$

where the total flow per unit width that passes through the cross-section is equal to the product of the Darcy velocity and the saturated thickness. Considering fixed hydraulic head at the left and right boundaries, h_L and h_R, the last equation admits the following simple analytical solution, often referred to as Dupuit approximation,

$$h^2(x) = ax^2 + bx + c \qquad (5)$$

where the constants a, b and c depends on K, R, the length of the domain (L^*), and the value of h at both boundaries (Haitjema, 2006; Bear, 2012). Therefore, h which also represents the position of the water table, depends non-linearly on the parameters of the problem and the position along the cross-section. It is possible to extend the solution to heterogeneous aquifers imposing continuity of hydraulic head and fluxes across the interface between different materials (Appendix A).

Although the Dupuit approximation is a reasonable approximation for many cases, it fails to account for the resistance in vertical flow that can occur in thick unconfined aquifers and anisotropic porous media with higher vertical than horizontal flow resistance ($K_v/K_h < 1$).

The Dupuit approximation is valid when $L^* \ll \hat{H}\sqrt{\frac{K_h}{K_v}}$, where $\hat{H}$ [L] is the effective saturated thickness. For isotropic porous media, the condition simplifies to $L^{*} \leq 5\hat{H}$ (Haitjema, 2006). In the next section, we use the Dupuit solution as an alternative modeling approach to estimate the water table for simple cases and compare it to the numerical solutions.

We consider the example problem depicted in Figure 2, which corresponds to an unconfined aquifer connected to two rivers that act as prescribed hydraulic head boundary conditions. Figure 3 shows the water table calculated with the analytical solution based on the Dupuit approximation in equation 5 assuming a homogeneous and a heterogeneous aquifer for different recharge rates considering the parameters listed in Table 1. As previously explained, the analytical solution is only valid for cases that satisfy the assumptions considered to derive it. Nevertheless, it provides a reasonable first-order approximation for other cases and can be used to perform a qualitative assessment or for comparison of the water table under different conditions. The position of the water table rises with higher recharge. For high recharge the water table has a water divide that is located almost at the middle point of the aquifer for the homogeneous aquifer, and at almost the middle point of the lower permeability section of the aquifer for the heterogeneous case. For the highest recharge equivalent to 365 mm/yr, the mounding of the water table is of the order of a few meters for the homogeneous aquifer, while it reaches more than 40 meters in the case of the heterogeneous aquifer. Such large variation on the elevation of the water table within a relatively short distance produces steep gradients that may be difficult to simulate with coarse numerical grids, e.g. > 10 m.

Table 1: Parameters of the example problem shown in Figure 3 considered in numerical simulations.

Parameter	Value	Unit
Aquifer length, **L**	1000	m
Aquifer height, **H**	80	m
Left hydraulic head, $\mathbf{h_L}$	5	m
Right hydraulic head, $\mathbf{h_R}$	10	m
Position interface, $\mathbf{x_K}$	600	m
Hydraulic conductiviy left, $\mathbf{K_1}$	1.00	m/d
Hydraulic conductiviy right, $\mathbf{K_2}$	0.01, 1.00	m/d
Anisotropy, $\boldsymbol{\alpha_{VH}}$	1.0, 0.5, 0.3, 0.1	-
Recharge rate, **R**	1e-4, 1e-5, 1e-3	m/d

Numerical solution

MODFLOW is based on a finite volume formulation to solve the partial differential equation (1). The latest version, MODFLOW 6, uses a 3D numerical grid that is composed of rectangular or irregularly shaped cells distributed in one or multiple layers (Langevin et al. 2017). The numerical solution is based on computing fluxes between adjacent cells as shown in Figure 4. In the standard form, the flux between two cells, e.g. cells c_i and c_j, is computed as the product of an overall factor that represents the capacity of the medium to carry water, referred to as conductance, and the head difference between the center points of adjacent cells, computed by a first-order finite difference approximation. MODFLOW 6 also includes a more sophisticated XT3D formulation to represent full 3D anisotropy (Provost et al., 2017); however, that formulation is not used in this work. The solution of the non-linear equation (equation 1) is based on a Picard iterative procedure, i.e. given an initial value for the hydraulic head at each cell, fluxes are evaluated and substituted in equation 1 and mass balance is checked. Values of h and the conductance values that depend on h are updated and the procedure is repeated until a closure criterion is satisfied.

For unconfined aquifers that can become dry or for unconfined aquifers that are represented with multiple layers, the underlying saturated formulations in MODFLOW require special attention. In the simplest case, MODFLOW will deactivate any cell with a calculated head that is below the cell bottom. This deactivation can occur during the solution procedure before the model has converged. Deactivated cells do not receive recharge or other flows and act as an impermeable barrier to flow. This behavior of a deactivated cell is often an unintended consequence of cell drying and may go unnoticed by an inexperienced user. Cells that start dry or cells that become dry during the simulation remain dry for the rest of the simulated period. Such situations often happen in transient problems when the water table falls with time. Drying conditions can also be encountered during the solution of steady-state problems that start with an initial guess for the water table position that is modified as part of the computation of the hydraulic head distribution. MODFLOW includes an alternative and optional ad-hoc approach to rewet dry cells based on the simulated head in surrounding cells (McDonald et al., 1992). The rewetting is controlled by a few parameters that indicate when a dry cell should be converted into a wet cell and vice versa (see Langevin et al., 2017 for MODFLOW 6 implementation details). The optimal values of those parameters are known to be problem dependent, hence the application of such procedure often ends in failure and solutions that are contaminated by spurious numerical artifacts. Typical problems that are found include oscillations in the head solution due to a dry cell being converted to wet at one iteration, and then reconverted back to dry in the next iteration. We refer to this MODFLOW solution option as the wet/dry or non-Newton approach.

Following approaches described by Painter et al. (2008) and implemented in MODFLOW-NWT (Niswonger et al., 2011) and MODFLOW-USG (Panday et al., 2013), MODFLOW 6 implements a similar Newton approach to estimate the position of the water table in unconfined aquifers, which is based on three key numerical improvements over the non-Newton approach. First, it uses a Newton-Raphson formulation instead of the Picard formulation to linearize the terms in equation 1 that depend on head. Second, it uses an upstream-weighted evaluation of the inter-cell conductance (calculated as the fully saturated conductance multiplied by the upstream cell saturation value) for horizontal cell connections. This upstream weighting preferentially allows water to flow into dry cells while restricting the flow of water out of cells that are dry or nearly dry. Third, all cells in the model domain are treated as active even if the simulated hydraulic head is lower than the elevation of the cell bottom (which was previously used as criterium to mark dry cells as inactive). The result of this Newton formulation is that flow (such as recharge or lateral flow) into a dry cell is instantaneously routed downward to the first cell that is not dry. We refer to this numerical algorithm as the Newton formulation. The Newton formulation has generally been shown to be more reliable than the wet/dry approach for solving the position of the water table.

The numerical solution for the example problem depends on two additional parameters: the horizontal and vertical grid discretization, which are equivalent to the number of columns and layers in the numerical grid. With the constant problem dimension, many columns result in grid cells with small spacing, hence higher numerical resolution. The same applies for the vertical discretization, which is controlled by the number of layers. In the limiting case of a grid with one layer, the numerical solution computed with MODFLOW solves equation 2, hence it should converge for fine horizontal numerical discretization to the Dupuit approximation. In this case, the numerical solution does not represent vertical resistance to flow and, is thus consistent with the Dupuit approximation.

Numerical simulations

Setup

We use MODFLOW 6 (version 6.2.2; Langevin et al. 2021) to estimate the position of the water table for the example problem depicted in Figure 2. Since the position of the water table depends on all the parameters that define the problem, i.e. recharge rate, aquifer length, boundary conditions, hydraulic conductivity, user-provided initial head to start iterations, etc; and the numerical parameters such as grid resolution in the horizontal and vertical directions; it is not possible to cover the full range of potential outcomes within a reasonable computational effort. Therefore, we consider only three parameters to perform a sensitivity analysis of the numerical solution: the recharge rate R, the grid discretization in the horizontal and vertical directions specified as the number of columns along the aquifer and layers, and the anisotropy of the materials computed as the ratio between the vertical and horizontal hydraulic conductivity, $\alpha_{vh} = K_v / K_h$. We consider recharge rates that are within typical values for semi-arid (36.5 mm/year) and wet (365 mm/year) climates (Scanlon et al, 2006). We consider anisotropy values (> 0.1) that are greater in comparison to typical values used in practical applications (as low as 0.01 or 0.001); however, they provide a good approximation to the changes in the results that can be expected due to this parameter. We consider only the case of a heterogeneous aquifer with values of horizontal hydraulic conductivity equal to 1.00 and 0.01 m/d for the left and right sections of the domain, respectively. We ran only steady-state simulations that required a few seconds to finish. The values of all parameters considered for the numerical solutions are listed in Table 1. For all simulations we set the initial head above the elevation of the ground surface to prevent starting a simulation with dry cells.

We consider different grid sizes defined by the number of columns between both rivers between 11 and 101 (i.e. horizontal cell size between 100 and 10 m), and horizontal layers between 1 and 80 (i.e. vertical cell size between 80 and 1 m). This level of grid discretization is on the order of the resolution used for many practical problems; hence the results of the numerical simulations provide a good representation of the level of accuracy that can be expected for these kinds of problems. It is expected that the numerical solution should converge to the true solution of the problem as the horizontal and vertical discretization is refined provided that the numerical algorithm is stable and consistent. For this particular example, we can compare the numerical estimation of the water table to the analytical solution provided by the Dupuit approximation. The Dupuit approximation was extended to the heterogeneous aquifer case and provides a reasonably good approximation for the dimensions considered for the problem and for low recharge rates and isotropic materials. For other cases, i.e. high recharge rates and/or anisotropic aquifers with higher vertical than horizontal flow resistance, the Dupuit approximation deviates from the true solution of the problem, which is expected to be better approximated by the numerical solution when the vertical discretization is sufficiently refined.

The numerical estimation of the water table position with MODFLOW 6 can be performed using the Newton-Raphson formulation or the non-Newton wetting/drying approach. We use both options to compare their ability to provide reasonable solutions for the example problem and to assess their robustness and stability. The settings for the linear and non-linear solver were specified with the parameter values listed in the Supporting Information. For many groundwater models, tuning of solver parameters is done in a haphazard manner by testing different solver parameters until a successful combination is identified. MODFLOW 6 has three pre-configured solver settings (SIMPLE, MODERATE, and COMPLEX) that can be selected based on a user understanding of how difficult the problem is to solve. Similar keyword settings are also available for MODFLOW-NWT and MODFLOW-USG. Alternatively, the user can individually set each solver parameter. Ideally, solver parameters are tuned based on the behavior of the numerical solution, which can optionally be written to simulation output files. Linear solver parameters should be adjusted when the inner iteration loop is not converging or is taking longer than expected to solve. The non-linear solver parameters should be adjusted when the head solution oscillates or converges slowly from one outer iteration to the next.

The combination of the two parameters considered for sensitivity analysis (three values of R and four values of α_{vh}) in combination with the different grid resolution (10 number of columns and 5 number of layers) results in a total of 600 different numerical simulations or runs. A relatively small number of the runs failed to converge according to the preset criteria (see details in Supporting Information) and, hence, were discarded. To improve the convergence of the numerical solver, we increased the maximum allowed number of inner iterations from 20 to 100 resulting in another 600 runs for a total of 1200 simulations. Such large numbers of simulations required relatively small computational effort and were run on a standard desktop PC within a few minutes. The pre- and post-processing of the simulations were automated with Python scripts using the FloPy library (Bakker et al., 2016), which has full support for MODFLOW 6. Summary tables that include information about convergence and differences between both the numerical and analytical solutions, and figures that show the estimated water table for all simulations are included in the accompanying Supporting Information.

Results

As a base case scenario, we consider an aquifer that includes only isotropic materials ($\alpha_{vh} = 1.0$) and the lowest recharge rate $R = 1\cdot10^{-4}$ m/d equivalent to 36.5 mm/year. Figures 5 to 8 show the estimated water table using different numerical grids with different resolution in the horizontal and vertical directions. For this base case scenario the Dupuit approximation provides a good representation of the water table position, hence it is expected that the numerical solution should be similar provided that enough spatial resolution in both horizontal and vertical directions is included. Figure 5 shows the computed water table considering the coarsest numerical grid. Although both numerical solutions are similar to the analytical solution, there are still considerable differences in the magnitude of the simulated elevation of the water table. Figure 6, which shows results for the highest horizontal resolution and lowest vertical resolution, demonstrates that the difference between the numerical and analytical solutions decreases as the horizontal resolution increases. Conversely, Figure 7 shows that more refined vertical resolution does not provide the same level of improvement in the numerical solution as the one obtained by decreasing the horizontal discretization. Finally, Figure 8 demonstrates that the numerical solution converges toward the true solution provided that enough spatial resolution in both directions is considered. This figure shows that for this case the pressure distribution is nearly hydrostatic, which results in almost vertical equipotentials that satisfy the assumptions considered for the derivation of the Dupuit approximation; hence, the water table position for this scenario is well represented by the Dupuit approximation.

Figure 9 shows the estimated mounding of the water table due to recharge, computed as the difference between the maximum elevation of the water table and the right boundary condition, versus the horizontal grid resolution for the lowest and highest recharge rates. For the lowest recharge, increasing horizontal resolution results in decreasing calculated mounding that converges toward three unique final values for all three number of layers (vertical resolution) shown. The convergence toward a single value (for each vertical resolution) seems to start for relatively coarse horizontal resolution (40 columns), which indicates that the numerical solution effectively converged. For the case of highest recharge, the simulated mounding increases with the horizontal grid resolution without reaching a clear asymptotic value, indicating that the numerical solution did not reach convergence since additional increases in the vertical resolution would likely result in further changes in the simulated value. The differences in the simulated mounding due to only horizontal grid resolution are approximately 50 cm for the lowest recharge and 1.5 m for the highest recharge. Furthermore, finer vertical resolution (higher number of layers) results in a difference of more than 2 m in the simulated mounding for the highest recharge rate. This is a consequence of the non-hydrostatic pressure distribution that occurs for that case, which results in a significant vertical gradient (as shown in the Supporting Information Figure S249). This vertical component of flow can only be represented if sufficient vertical discretization is included. The magnitude of the difference for different vertical resolution can be important for some applications that require comparing observed and simulated hydraulic heads.

For the highest recharge rate, the Newton formulation provides a solution that is closer to the Dupuit approximation and that results in a relatively small increase in the prescribed hydraulic head at the right boundary in comparison to the Non-Newton (wetting/drying) approach. The fact that the simulated hydraulic head at the right boundary is not exactly equal to the prescribed value is the result of the simplification of the real problem for its numerical solution. In the real world, a high recharge rate would produce a rising water table that would result in the occurrence of seepage flows on the right boundary above the hydraulic head specified by the water elevation in the river. It is difficult to represent naturally occurring groundwater discharge through a seepage face with a saturated groundwater model such as MODFLOW.

Figure 10 shows the difference between numerical solutions computed with a single layer grid and analytical approximations versus recharge rate. The differences between the Newton (N), Non-Newton (NN) and analytical (D) solutions are labeled N-D, NN-D and N-NN. Holding other parameters constant, increasing recharge results in larger differences between both numerical solutions. The numerical solution computed with the Newton solver deviates more from the analytical solution than the Non-Newton solution, which differs by less than 5 cm for the highest horizontal resolution grid (ncol = 101). When using a single model layer, the numerical solutions should closely match the Dupuit analytical solution because neither represent vertical resistance to flow. Results from the Newton formulation are not as accurate as the Non-Newton wetting/drying simulation, because the Newton formulation uses an upstream weighting approach, which causes a bias in the solution. Upstream weighting results in an effective aquifer transmissivity that is larger than what would be calculated using an arithmetic average of saturated thickness. The effect of this bias decreases as the horizontal resolution increases.

The Newton formulation results in smaller differences than the Non-Newton formulation compared to the analytical solution when the numerical grid is refined in the vertical direction (larger number of horizontal layers). This is evident by comparing the Newton, Non-Newton, and Dupuit results in Figure 11. The difference between Newton and the Dupuit approximation increases with increasing recharge rates as a consequence of the higher mounding of the water table. For the highest resolution numerical grid, the Newton formulation has more simulations that do not converge than the Non-Newton formulation. Although the Newton formulation appears to provide a reasonable estimation of the water table position for scenarios that result in higher mounding, a closer inspection reveals spurious oscillations near the water table with isolated dry cells, which explains the convergence failure (see figures included in the Supporting Information for details).

Lower anisotropy ratios, i.e. higher vertical flow resistance, result in a higher water table due to the increased mounding that is required to allow the recharged water to flow towards the boundaries of the aquifer. Figures S230, S280, S530 and S580 in the Supporting Information show a simulated water table for a 101-column and 20-layer grid considering the highest recharge rate (365 mm/yr) for decreasing anisotropy ratios equal to 1.0, 0.5, 0.3 and 0.1, respectively. An analysis of the results of those simulations indicate that: i) the numerical solution computed with the Newton solver failed to converge due to numerical instability near the water table that produced isolated dry cells (seen as white spots near the right side in the upper graph), ii) increasing vertical flow resistance results in flooding of the cells above the right boundary due to the increased mounding required to generate strong vertical gradients to carry the recharged water towards the outlet boundaries located at both sides of the model domain, and iii) lower anisotropy ratios result in increased mounding, more flooding near the right boundary, and larger differences between the numerical and analytical. For the lowest anisotropy ratio, it is interesting to note the differences between both numerical solutions and the analytical approximation near the right boundary (e.g. Figure S530). While the Dupuit approximation honors the prescribed hydraulic head, both numerically simulated water tables show a much higher hydraulic head in the cells above the highest cell that represents the boundary condition. It is also interesting to note the appearance of cells with apparent perched conditions near the left side of the low permeability part of the domain for the low values of α_{vh} simulated with the Newton solver. Such perched conditions are more evident in the equivalent scenarios that consider lower recharge rates. The appearance of perched conditions and the presence of isolated dry cells partially explains the convergence difficulties of the Newton formulation for scenarios with large water table mounding, i.e. low α_{vh} and/or higher recharge rate (see figures and tables in Supporting Information for a detailed summary of results and convergence of all numerical simulations).

In some situations, the solution computed with the Non-Newton formulation using the default settings for the numerical solver result in anomalous solutions (see examples in the Supporting Information). Even if those solutions are reported as converged and have a perfect mass balance with near zero error, they are wrong and far from the correct solution. In one case, the Non-Newton formulation resulted in dry cells for a large section of the model domain. For the Non-Newton formulation, once all the cells in a vertical column are dry, MODFLOW no longer applies recharge to that column because no active cells exist.

Thus, while these results are considered to be numerically converged, the results are nonsensical and should not be used for analysis. Other results presented in the Supporting Information further illustrate potentially erratic and incorrect behavior within the Non-Newton formulation.

Figure 12 shows a case for which the Newton solver using the default numerical settings fails to provide reasonable solutions for the water table. For this particular case, the solution did not converge, and thus the computed water table is not accurate, and the reported mass balance error is above 60%. Such failed cases were relatively uncommon for the simulated scenarios representing less than 15% of all runs. In an attempt to improve convergence for this problem, we increased the number of inner iterations for the linear solver from 20 to 100. Figure 13 shows the solution computed with the higher number of iterations, which although closer to the expected solution still fails to converge and shows some numerical artifacts near the interface between both materials at $x = 600$ m. The mass balance error for the simulation shown in Figure 13 was less than 3%. Hence, the spurious artifacts presented in Figure 13 should be considered as a warning about using the option provided by MODFLOW to continue running despite not reaching convergence. Such an option, which is very useful for some challenging problems, should always be used with care and the computed solutions should be verified and validated by other means. Further increases in the maximum number of inner iterations up to 600 did not improve in the numerical solution but resulted in a lower mass balance error equal to less than 2%, which is even closer to the common threshold limit of 1%. Therefore, we consider that the scenario presented in Figures 12 and 13, highest recharge and lowest anisotropy, represents a difficult problem for MODFLOW that tests the limits of the Newton formulation.

Moreover, the results of all runs demonstrated that the Newton formulation tends to be less reliable than the Non-Newton formulation for similar problems (i.e. high recharge, low anisotropy and fine grid discretization), resulting in a higher number of runs that did not converge in comparison to the traditional wet/drying approach (Table S2).

Conclusions

The numerical estimation of the water table position in unconfined aquifers with saturated flow simulators is challenging and prone to numerical instabilities. Challenges arise due to the non-linear behavior of the partial differential equation that must be solved, such as instabilities that can occur when applying MODFLOW traditional wetting and drying methods and difficulties to approximate the shape of the water table with fixed finite grid size. The latter problem is particularly important when the water table has steep gradients, as in the case of the example problem analyzed in this article.

Conclusions that derive from the analysis of the results of the numerical simulations presented above, are:

a) For a single layer model, the MODFLOW solution and the analytical solution based on the Dupuit approximation are similar, independently of the other parameters provided that sufficient horizontal resolution is considered in the numerical grid.
b) Adding more vertical resolution to the numerical solution, i.e. using more layers, can result in significant changes in the solution for cases where vertical resistance to flow is important, e.g. high recharge rates or low anisotropy ratios for the example problem.

c) MODFLOW's Newton formulation generally provides accurate solutions when the grid contains more than one layer and does not suffer from the Non-Newton convergence issues related to the wetting and drying of cells. However, the Newton formulation may result in higher percentages of non-converging simulations under some conditions.

d) The numerical solution and its numerical stability may be highly sensitive to the value of some of the physical input parameters that define the problem, e.g. recharge rate and anisotropy ratio. Convergence behavior is also sensitive to numerical settings such as maximum number of inner and outer iterations for the non-linear numerical solution. Finding optimal values for all those parameters that in combination guarantee a robust numerical solution can be problematic and may require sophisticated strategies for optimizing solution parameters (Newcomer and Hunt, 2022).

e) Changes in numerical parameters such as grid resolution and settings for the linear and non-linear solutions can result in differences of up to several meters for the calculated water table for the example problem used here. Therefore, similar application scenarios should expect a degraded level of accuracy.

The computation of the water table through numerical simulations can be the only choice for problems that consider significant vertical gradients that result in non-hydrostatic pressure distribution. However, the Dupuit approximation provides a reasonable solution for a large set of cases and, it is also considerably easier and faster to evaluate. Therefore, both types of solutions, numerical and analytical, should be seen as complementary for the estimation of the water table in unconfined aquifers.

When using numerical simulations to estimate the position of the water table it is advisable to: i) verify that the grid resolution is adequate for the desired level of accuracy by conducting a grid convergence study, which requires using different numerical grids to compute solutions for the same input parameters, ii) compare solutions computed with different methods, e.g. Newton versus Non-Newton or Dupuit versus Newton, to understand the main properties of the solution at hand; iii) ensure that the numerical solution is free of numerical artifacts, which can be best performed by simple visual inspection; iv) verify that all boundary conditions are reasonable, particularly with respect to the potential occurrence of phreatic springs, and v) for situations where vertical resistance to flow is important it may be necessary to try both the Newton and Non-Newton formulations to determine which one works best for a particular problem.

The convergence difficulties encountered for some example problem configurations remains a challenge for these types of numerical analyses. The work here highlights the difficulties that might be expected when running a sensitivity analysis over a wide range of conditions or when applying a parameter estimation program. Though we did not systemically address convergence problems in this paper, we found that it is best to avoid the pre-configured solver settings available in MODFLOW. Instead, we found it was best to start with the simplest configuration and turn on more sophisticated settings only as necessary based on solution behavior. This is achieved most efficiently by developing an understanding of the difference between inner and outer iterations, properties of the underlying matrix equations and how they are affected by MODFLOW formulations and options, and the role of non-linearity in complicating the solution process. Many of these solution concepts are described for MODFLOW 6 by Hughes et al. (2017).

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Supporting Information

Additional Supporting Information may be found in an online document that contains Figures S1 through S601 and Tables S1 through S2 as referenced in the text.

Supporting information is generally not peer reviewed.

Appendix A: Dupuit approximation for heterogeneous aquifer

Considering a heterogeneous aquifer composed of two materials with hydraulic conductivity K_1 and K_2 as depicted in Figure 2, we can apply equation 5 to both sides of the interface located at x_K,

$$h^2(x) = a_1 x^2 + b_1 x + c_1 \qquad x \le x_K \tag{A.1}$$

$$h^2(x) = a_1(x - x_K)^2 + b_1(x - x_K) + c_1 \quad x > x_K \tag{A.2}$$

Equations (A.1) and (A.2) include six coefficients. Two can be readily evaluated: $a_1 = - R/K_1$ and $a_2 = - R/K_2$. The other four can be evaluated by imposing both boundary conditions at the left and right boundaries and applying continuity of the hydraulic head and its derivative (flow rate) at the interface boundary:

$$h(x = 0) = h_1 \tag{A.3}$$

$$h(x = L) = h_2 \tag{A.4}$$

$$h\left(x = x_K^-\right) = h(x = x_K^+) \tag{A.5}$$

$$K_1 h h^{'}]_{(x=x_K^-)} = K_2 h h^{'}]_{(x=x_K^+)} \tag{A.6}$$

Then we can evaluate the remaining parameters to obtain:

$$c_1 = h_1^2 \tag{A.7}$$

$$c_2 = a_1 x_K^2 + b_1 x_K + c_1 \tag{A.8}$$

$$b_1 = (h_2^2 - a_2 y_K^2 - 2a_1\left(\frac{K_1}{K_2}\right)x_K y_K - a_1 x_K^2 - c_1)/(\frac{K_1}{K_2} y_K + x_K) \tag{A.9}$$

$$b_2 = \frac{K_1}{K_2}(b_1 + 2a_1 x_K) \tag{A.10}$$

where $y_K = L - x_K$.

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Figures

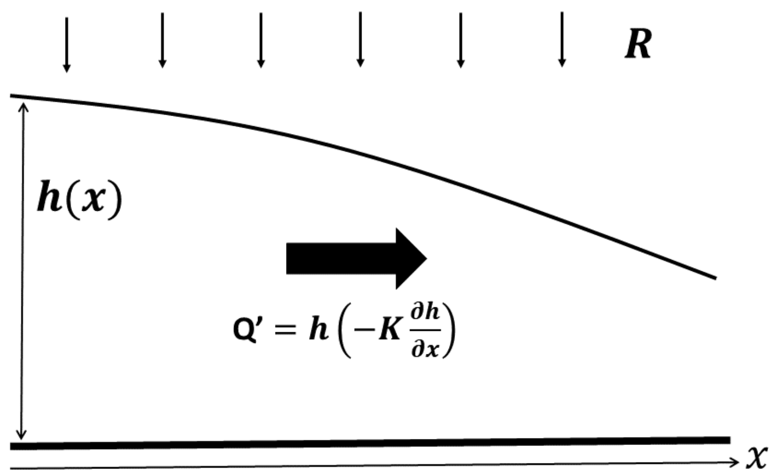

Figure 1: Schematic of unconfined aquifer cross-section with uniform recharge R. The flow per unit width of the, Q', aquifer depends on the hydraulic gradient $\partial h/\partial x$, hydraulic conductivity K and saturated thickness h assuming a flat aquifer bottom $\xi = 0$.

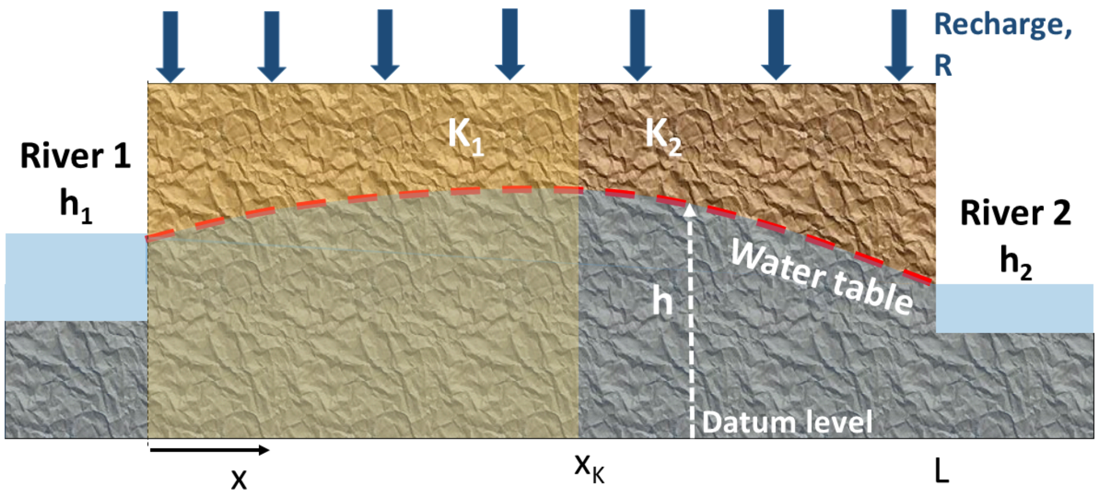

Figure 2: Schematic of the example problem. An unconfined aquifer of length L^* connected to two rivers with hydraulic head h_1 and h_2. The aquifer is composed of two materials with hydraulic conductivity K_1 and K_2 and an interface located at $x_K = 0.6L^*$.

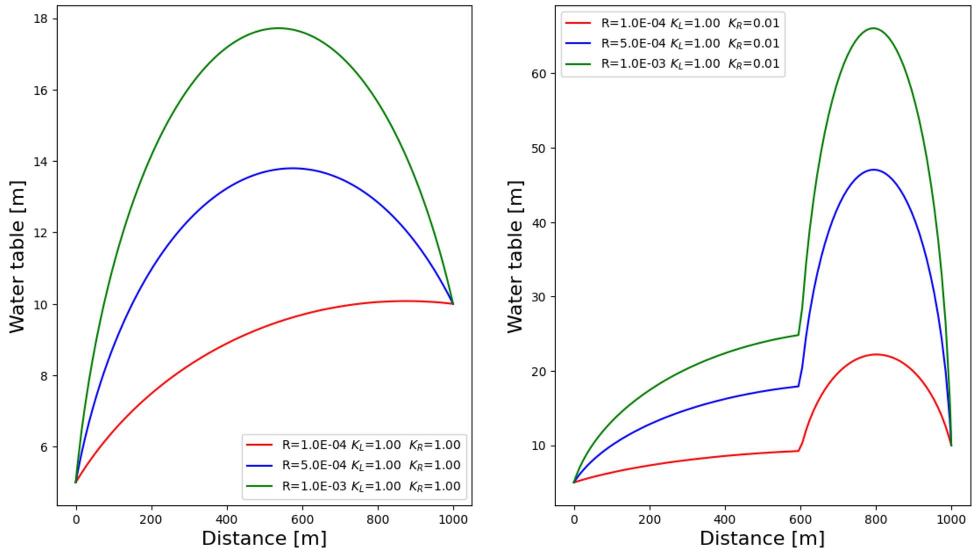

Figure 3: Water table estimated with Dupuit approximation considering the parameters listed in Table 1. Homogeneous (left) and heterogeneous aquifers and different recharge rates equal to $1x10^{-4}$ m/d (36.5 mm/yr), $5x10^{-4}$ m/d (182.5 mm/yr) and $1x10^{-3}$ m/d (365.0 mm/yr).

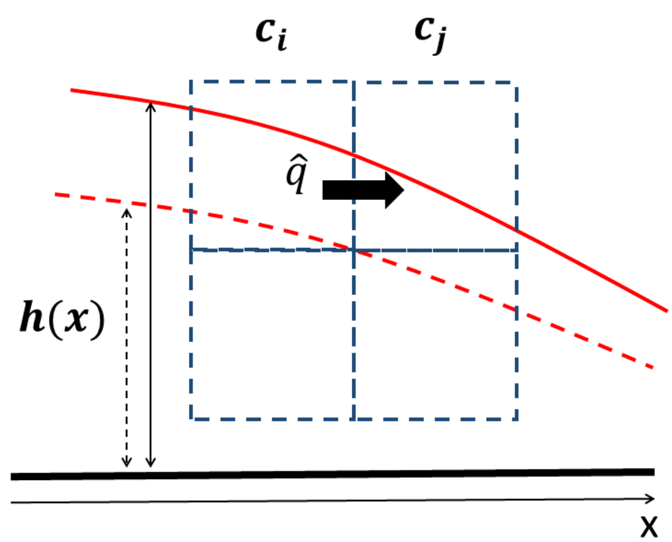

Figure 4: The numerical approximation of the flux $\hat{q}$ between cells c_i and c_j is prone to numerical instabilities due to changes in the position of the water table. When the water table (red line) coincides with the cell bottom (dashed line) the cell becomes dry and $\hat{q}$ becomes near zero. Different criteria and procedures have been proposed to allow the rewetting of dry cells and to calculate numerical fluxes to prevent numerical instabilities.

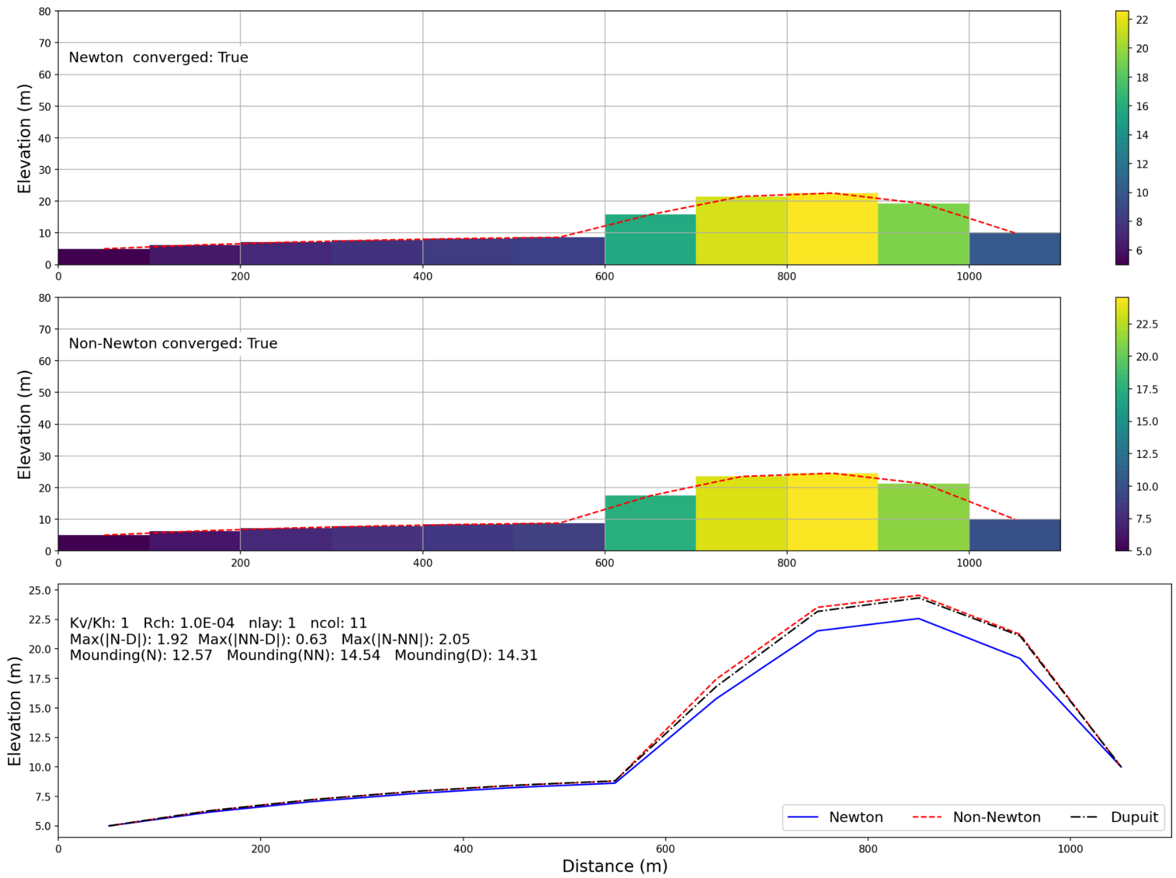

Figure 5: Simulated water table position for base case with coarsest numerical grid (11 columns) and coarsest vertical resolution (1 layer). Colors represent simulated hydraulic head in meters. Dashed red line in upper and middle plot shows position of water table defined as the maximum value of hydraulic head for each column. Solutions computed with Newton (upper) and Non-Newton (middle) solvers, and comparison between both numerical and the Dupuit solutions (lower).

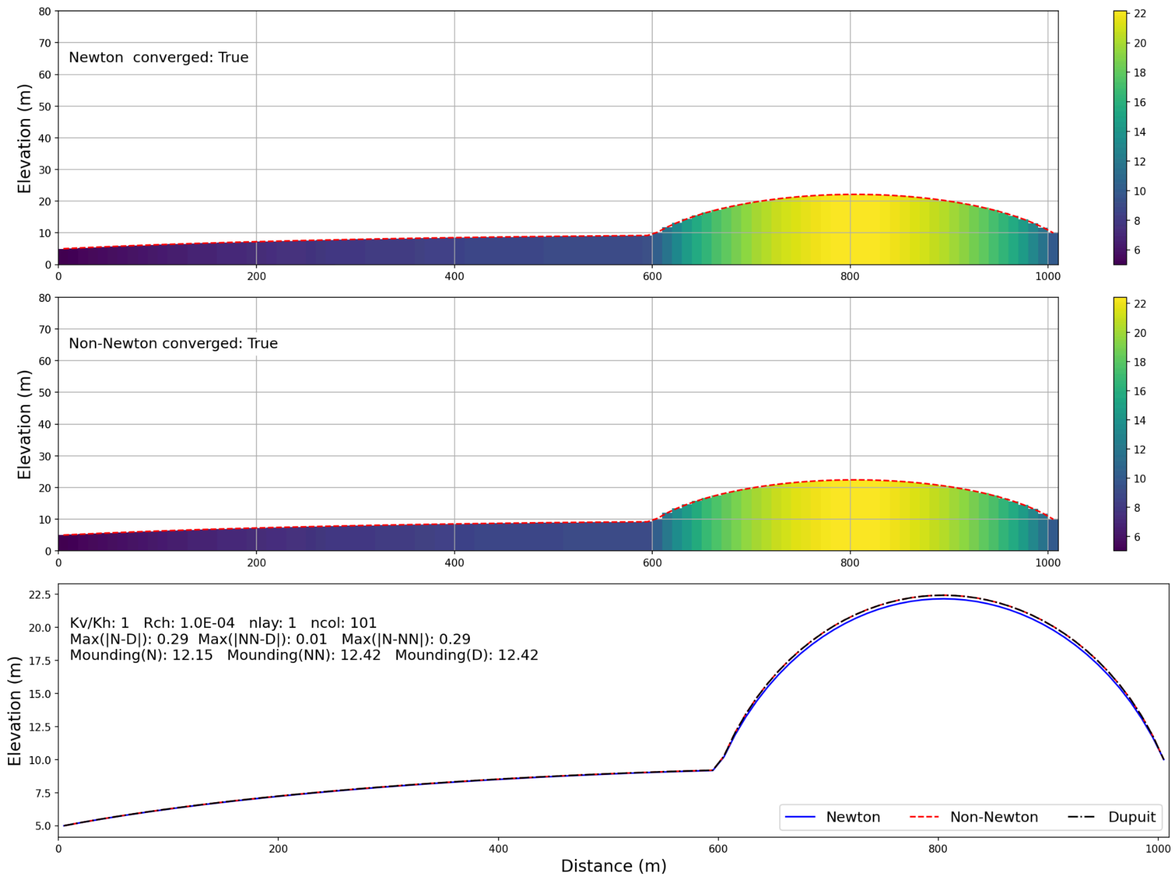

Figure 6: Simulated water table position for base case with numerical grid with finest horizontal resolution (101 columns) and coarsest vertical resolution (1 layer). Colors represent simulated hydraulic head in meters. Dashed red line in upper and middle plot shows position of water table defined as the maximum value of hydraulic head for each column. Solutions computed with Newton (upper) and Non-Newton (middle) solvers, and comparison between both numerical and the Dupuit solutions (lower).

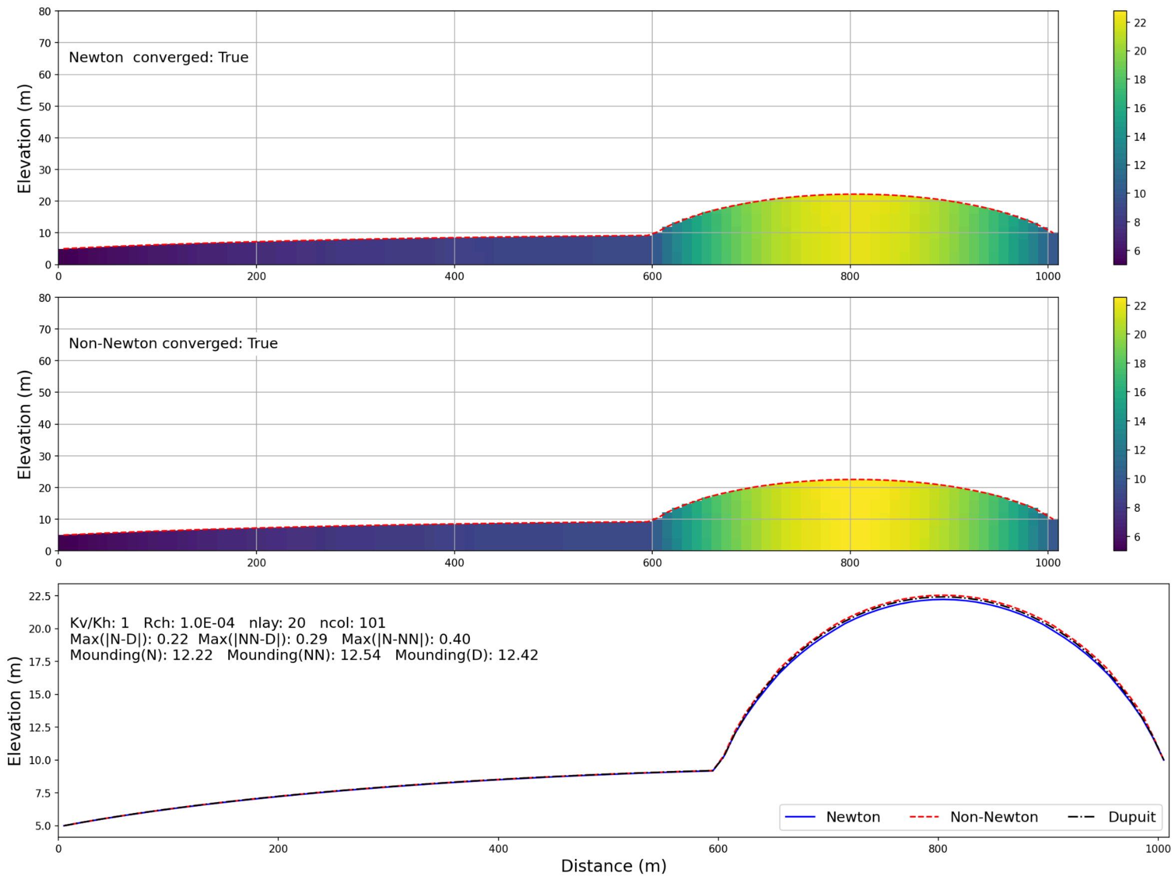

Figure 7: Simulated water table position for base case with numerical finest grid in the horizontal (101 columns) and improved vertical resolution (20 layers). Colors represent simulated hydraulic head in meters. Dashed red line in upper and middle plot shows position of water table defined as the maximum value of hydraulic head for each column. Solutions computed with Newton (upper) and Non-Newton (middle) solvers, and comparison between both numerical and the Dupuit solutions (lower).

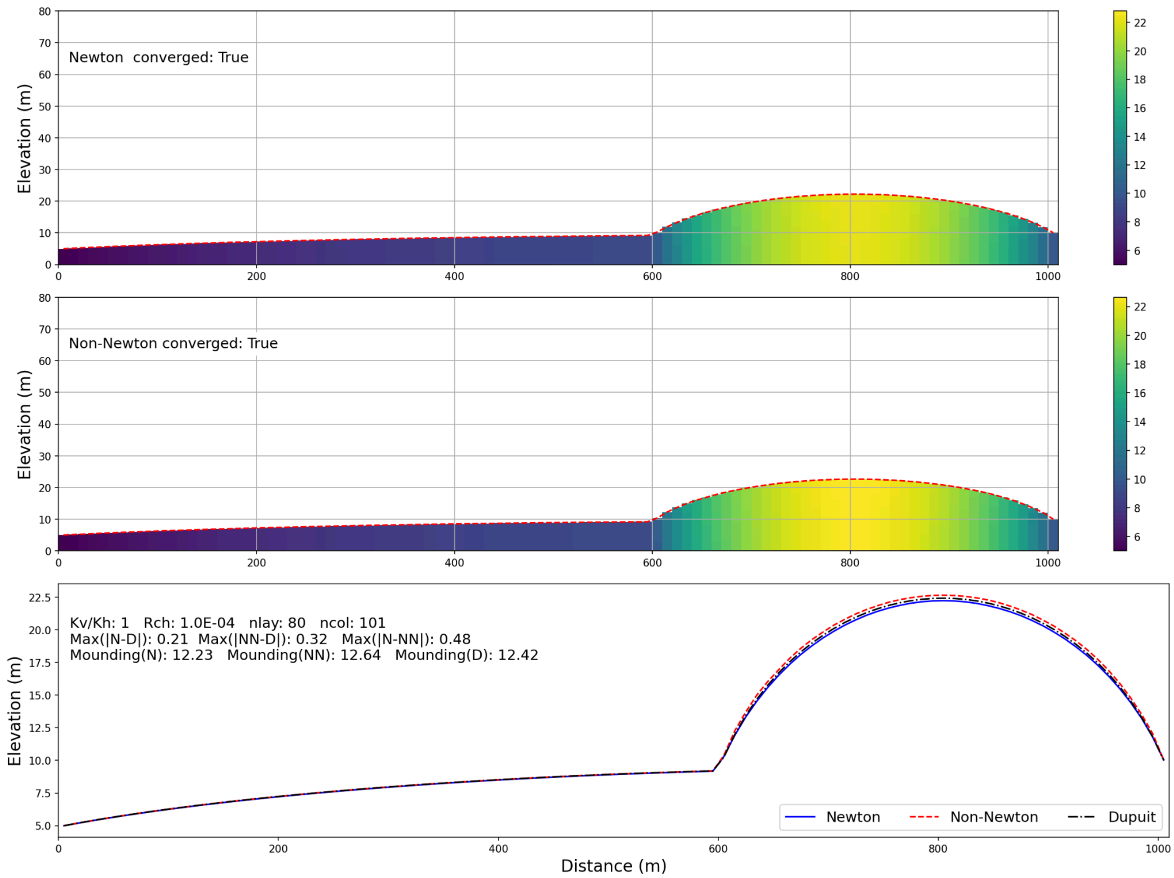

Figure 8: Simulated water table position for base case with finest numerical grid (101 columns and 80 layers). Colors represent simulated hydraulic head in meters. Dashed red line in upper and middle plot shows position of water table defined as the maximum value of hydraulic head for each column. Solutions computed with Newton (upper) and Non-Newton (middle) solvers, and comparison between both numerical and the Dupuit solutions (lower).

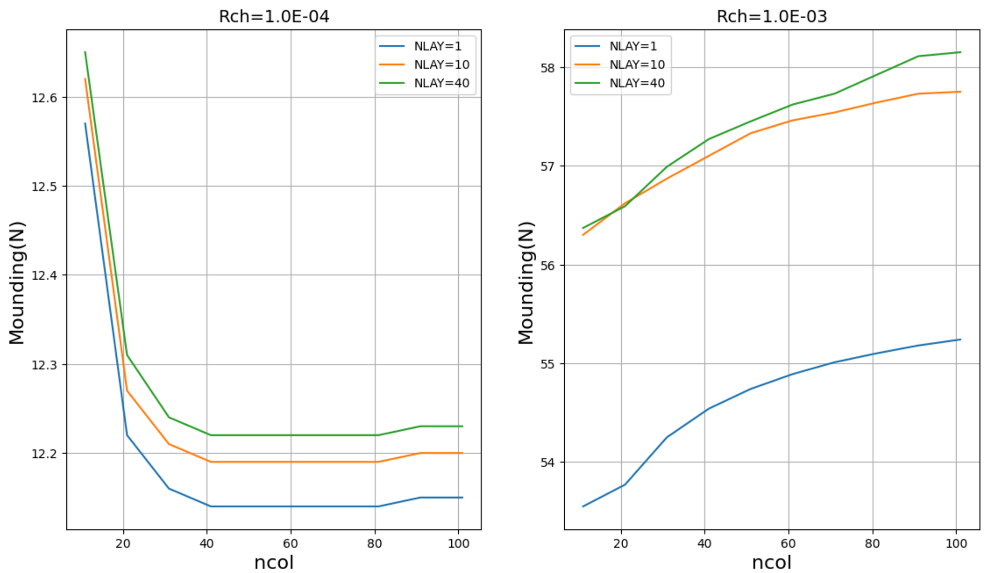

Figure 9: Estimated mounding, i.e. the difference between the maximum water table elevation and the right boundary condition, computed with the Newton formulation versus horizontal grid resolution for the lowest (left) R = 1.0E-04 m/d (36.5 mm/year) and highest (right) R = 1.0E-03 m/d (365 mm/year) recharge rates.

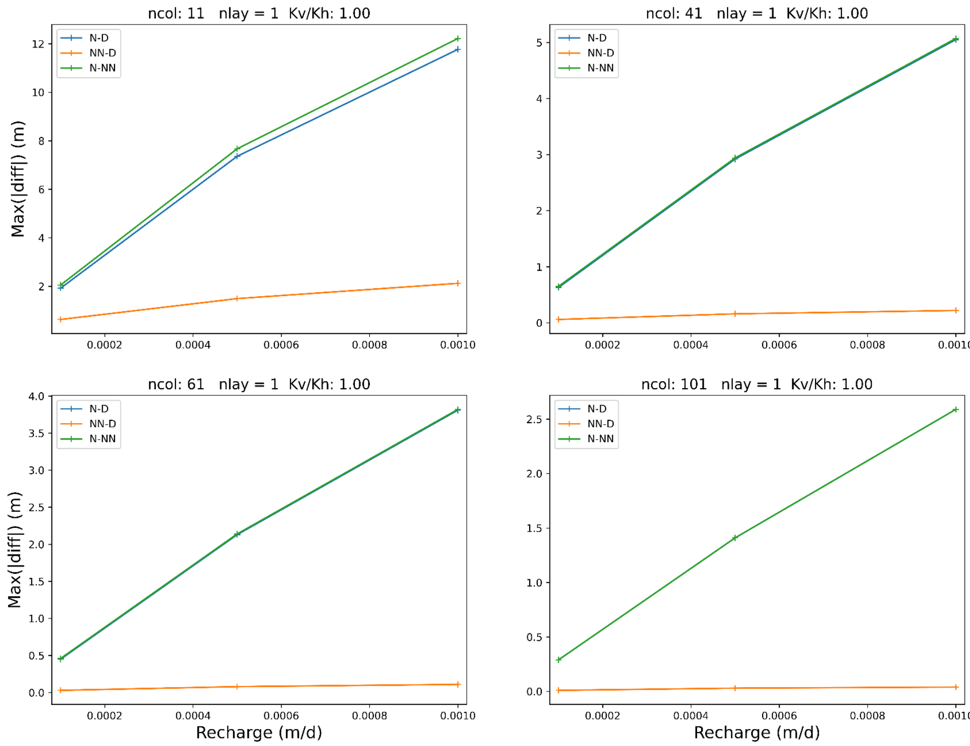

Figure 10: Difference between numerical solutions (Newton, N, and Non-Newton, NN) and Dupuit approximation (D) versus recharge rate for a single layer grid. Plots show results considering different horizontal grid resolution, i.e. number of columns (ncol). Increasing recharge results in an increasing difference between both numerical solutions (N-NN). However, the Non-Newton solution in a single layer grid is almost identical to the Dupuit approximation for fine horizontal resolution, i.e. large number of grid columns (ncol).

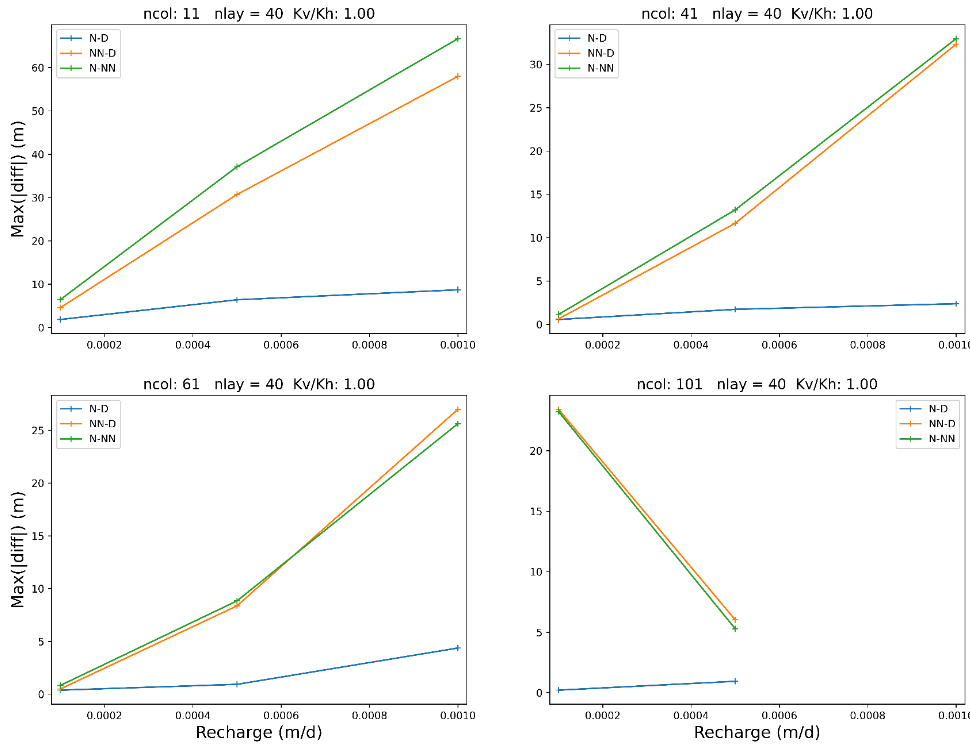

Figure 11: Difference between numerical solutions (Newton, N, and Non-Newton, NN) and Dupuit approximation (D) versus recharge rate for a 40 layers grid. Plots show results considering different horizontal grid resolution, i.e. number of columns (ncol). Increasing recharge results in an increasing difference between both numerical solutions (N-NN). The fine vertical resolution results in significant differences between both numerical solutions and the Dupuit approximation, which is not able to represent the strong vertical gradients and fluxes that occur for high recharge rates.

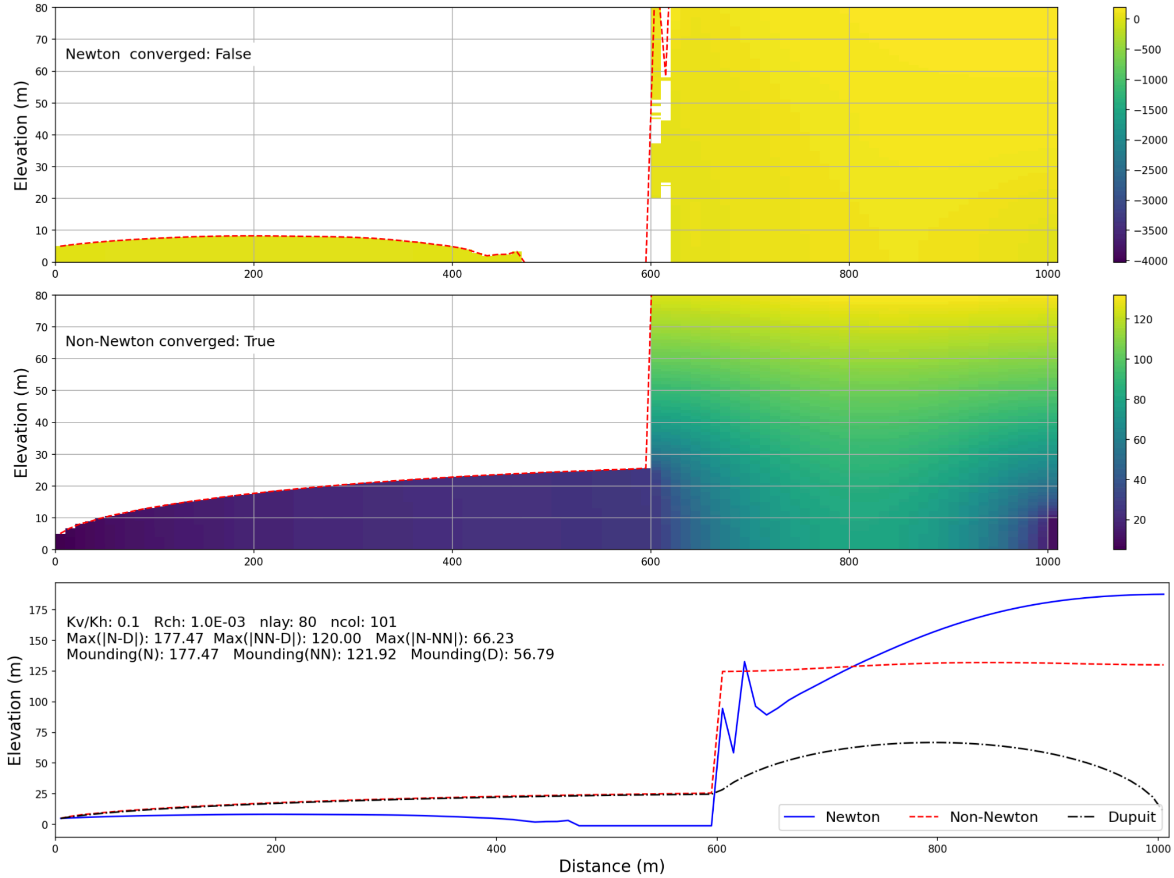

Figure 12: Simulated water table position for one of the settings with failed convergence considering default convergence settings. Colors represent simulated hydraulic head in meters. Dashed red line in upper and middle plot shows position of water table defined as the maximum value of hydraulic head for each column. Solutions computed with Newton (upper) and Non-Newton (middle) solvers, and comparison between both numerical and the Dupuit solutions (lower).

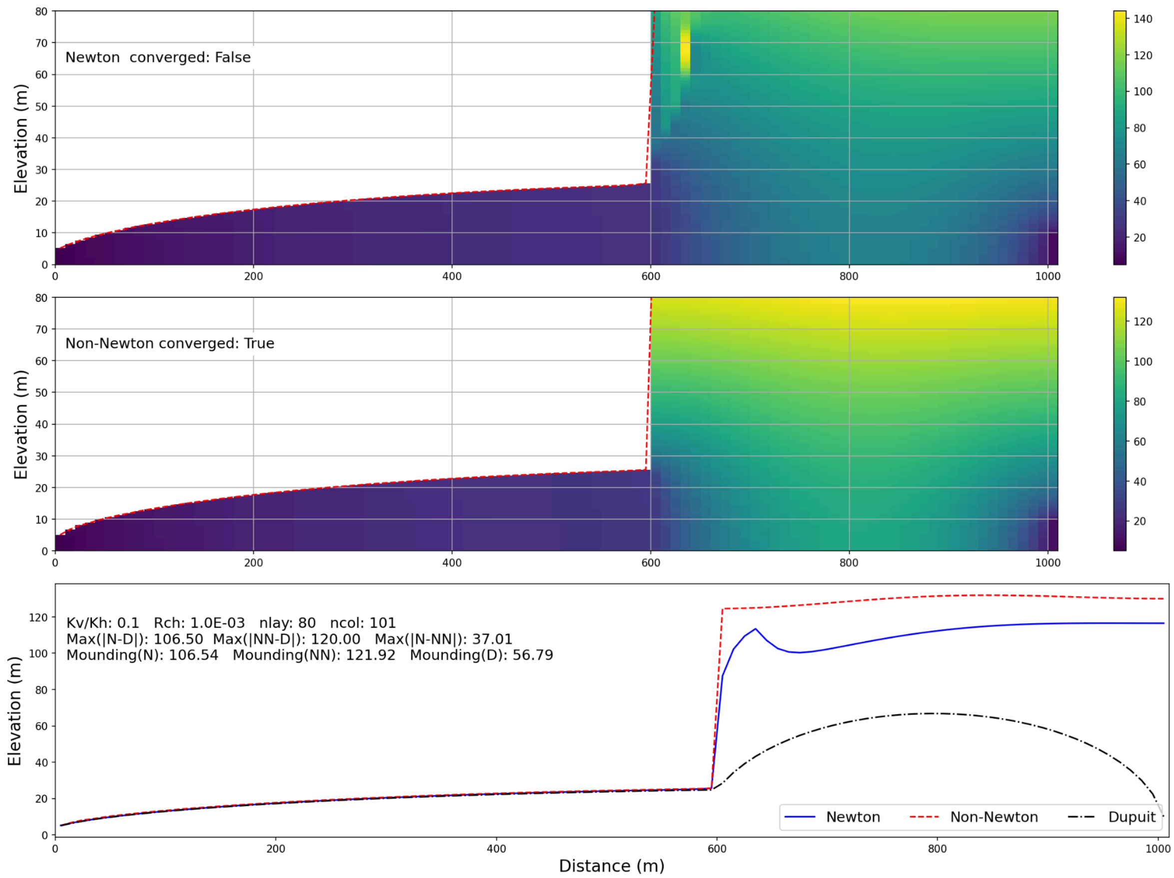

Figure 13: Simulated water table position for one of the settings (same as shown in Figure 12) with failed convergence considering increased convergence settings. Colors represent simulated hydraulic head in meters. Dashed red line in upper and middle plot shows position of water table defined as the maximum value of hydraulic head for each column. Solutions computed with Newton (upper) and Non-Newton (middle) solvers, and comparison between both numerical and the Dupuit solutions (lower).