Title

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Technical Notes

Core Ideas

- The coupling algorithm between HYDRUS-1D and MODFLOW is updated.
- Pressure head profiles are updated based on the groundwater table and bottom flux after each time step.
- This eliminates sudden variations in inflow and outflow fluxes with groundwater table changes.

Updating the Coupling Algorithm between HYDRUS and MODFLOW in the HYDRUS Package for MODFLOW

Sahila Beegum,* Jiří Šimůnek, Adam Szymkiewicz, K.P. Sudheer, and Indumathi M. Nambi

The HYDRUS-based flow package for MODFLOW (the HPM or the HYDRUS package) is an existing unsaturated zone flow package for MODFLOW. In MODFLOW with the HPM, the groundwater modeling domain is discretized into regular grids that can be combined into multiple zones based on similarities in soil hydrology, topographical characteristics, and the depth to the groundwater. Each of these zones is assigned one unsaturated soil profile (the HPM profile). In this model, after every MODFLOW time step, the flux at the bottom of the HPM profile is given as an input recharge flux to MODFLOW. MODFLOW simulates groundwater flow, and the water table depth at the end of the MODFLOW time step is assigned as the bottom boundary condition in the HPM profile. The current coupling algorithm assumes that the groundwater table in the HPM profile remains constant throughout the entire MODFLOW time step. This results in unrealistic sudden inflow and/or outflow fluxes at the bottom of the HPM profile after every time step. The objective of this study was to develop a methodology to eliminate the error in the determination of the recharge flux at the bottom of the HPM profile. This was achieved by updating or modifying the pressure head profile in the HPM profile after every MODFLOW time step. The effectiveness and the applicability of the new coupling algorithm were evaluated using different case studies. The new coupling algorithm is effective in eliminating unrealistic sudden variations in the bottom flux in the HPM profiles.

Abbreviations: 1D, one-dimensional; 3D, three-dimensional; HPM, HYDRUS Package for MODFLOW.

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In the past few decades, the coupling of one-dimensional (1D) unsaturated zone models with three-dimensional (3D) groundwater flow models to simulate various processes in and interactions between unsaturated and saturated soil zones has received a lot of attention. This is mainly because of the computational complexity and requirements of fully 3D variably saturated flow models when modeling larger domains with unsaturated soil zones (e.g., SHE model [Abbott et al., 1986], MODFLOW-SURFACT [HydroGeoLogic, 1996], FEFLOW [Diersch and Kolditz, 1998], TOUGH2 [Pruess et al., 1999], VSF [Thoms et al., 2006], HydroGeoSphere [Therrien et al., 2010], HYDRUS (2D/3D) [Šimůnek et al., 2016], MIN3P [Mayer et al., 2012], and PARFLOW [Maxwell et al., 2016]).

MODFLOW (Harbaugh et al., 2000) is a widely accepted 3D groundwater flow model. There have been many attempts to incorporate unsaturated zone flow models into MODFLOW (e.g., Havard et al., 1995; Facchi et al., 2004; Niswonger et al., 2006; Twarakavi et al., 2008; Lin et al., 2010; Zhu et al., 2011; Xu et al., 2012). The basic principle behind linking independent models for unsaturated and saturated soil zones is the exchange of information regarding the recharge flux from the unsaturated zone to the saturated zone and the elevation of the water table at appropriate time steps.

The HYDRUS-based flow package for MODFLOW (further referred to as the HPM or the HYDRUS package) was developed by Seo et al. (2007) and Twarakavi et al. (2008) to simultaneously evaluate transient water flow in unsaturated and saturated zones. In this package, the subroutines from the computational module of HYDRUS-1D

(Šimůnek et al., 2016) simulating unsaturated water flow in the vadose zone were coupled to MODFLOW (Harbaugh et al., 2000) simulating saturated groundwater flow. The HYDRUS package can represent the effects of unsaturated zone processes, such as infiltration, evaporation, root water uptake, capillary rise, and recharge in homogeneous or layered soil profiles. The coupled model is effective in addressing spatially variable saturated–unsaturated hydrological processes at the regional scale (Twarakavi et al., 2008). The most recent version of the HYDRUS package, which is available to the public, is compatible with MODFLOW-2005 (Harbaugh, 2005).

Governing Equations in MODFLOW and the HYDRUS Package

Groundwater flow is modeled in MODFLOW by solving the mass conservation equation using the finite difference approximation. The two-dimensional movement of groundwater of constant density in an unconfined aquifer is described by the partial differential equation (derived by applying the Dupuit assumption) as

$$K_x \frac{\partial}{\partial x}\left(H \frac{\partial H}{\partial x}\right) + K_y \frac{\partial}{\partial y}\left(H \frac{\partial H}{\partial y}\right) = S_y \frac{\partial H}{\partial t} \qquad [1]$$

where K_x and K_y are the hydraulic conductivities [L T^{-1}] in the x and y directions, respectively, H is the piezometric head [L], S_y is the specific yield (dimensionless) of the porous material, and t is time [T].

The HYDRUS package simulates water flow in the unsaturated zone using the modified one-dimensional Richards equation:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\frac{\partial h}{\partial z} - K(h)\right] - S \qquad [2]$$

where θ is the volumetric water content (dimensionless), h is the soil water pressure head [L], t is time [T], z is the vertical coordinate [L], S is a sink term [T^{-1}], and $K(h)$ is the unsaturated hydraulic conductivity [L T^{-1}]. The unsaturated hydraulic conductivity, $K(h)$, and the water content, $\theta(h)$, depend on the soil water pressure head. This makes the Richards equation a highly nonlinear equation that needs to be solved numerically. The HPM permits the use of five different analytical models to describe the soil hydraulic properties (i.e., Brooks and Corey, 1964; van Genuchten, 1980; Vogel and Císlerova, 1988; Kosugi, 1996; Durner, 1994).

Spatial and Temporal Discretization in the HYDRUS Package

In MODFLOW, the groundwater modeling domain is discretized into regular grids. These grids are combined into multiple zones based on similarities in soil hydrology, depth to the groundwater, and topographical characteristics. Each of these zones is assigned one vertical soil profile (the HPM profile) that extends from the soil surface down to a depth, which is below the deepest possible water table level that can occur during the simulation.

The total simulation period in MODFLOW is divided into stress periods (during which the external stresses such as pumping, recharge, or river stage remain constant), and each stress period is further divided into time steps. For each MODFLOW time step, the HYDRUS package simulates water flow in the unsaturated zone for each HPM profile. The HYDRUS package uses its own time stepping algorithm, based on user-defined criteria. Since the flow conditions in the vadose zone vary more rapidly than in the saturated zone, the HPM time steps are generally smaller than the MODFLOW time steps. The numerical solution of the nonlinear Richards equation also requires smaller time steps for simulating unsaturated zone flow.

Current Coupling Algorithm

The HPM simulates water flow in the unsaturated zone during a particular MODFLOW time step by considering the water table depth calculated by MODFLOW during the previous time step as the bottom boundary condition. When the HPM profile is associated with more than one MODFLOW grid cell, the average value of the water table position in these cells is used as the bottom boundary condition. The bottom flux calculated by the HPM during the current time step is passed to MODFLOW as a recharge flux to simulate the groundwater flow and to calculate the groundwater level change during the current time step. The bottom boundary condition thus changes stepwise in the HPM. See Seo et al. (2007) for more details.

Limitations of the HYDRUS Package

The current coupling algorithm implicitly assumes that the pressure head at the bottom of the HPM profile remains constant throughout the MODFLOW time step. This is less realistic when there is a large change in the water table level during this time step due to recharge from the unsaturated zone or due to some other lateral inflow into the saturated soil zone. In reality, the groundwater table varies continuously with time in response to vadose zone flow. A sudden change in the position of the groundwater table in the HPM profile after every MODFLOW time step leads to a change in the bottom boundary condition (a time-variable pressure head boundary condition). Since the bottom boundary condition does not at this moment correspond with the flow profile at the previous time step in the HPM profile, this results in a sudden inflow into the soil profile when the water table level is increased or a sudden outflow when the water table level is decreased. This results in the inaccurate estimation of the cumulative bottom flux throughout the duration of the simulation (Twarakavi et al., 2009; Kuznetsov et al., 2012).

Objectives

The main objective of this study was to eliminate sudden inflow or outflow fluxes at the bottom of the HPM profile when the groundwater table depth changes. This was achieved by updating the coupling algorithm between MODFLOW and the HPM. The second objective was to evaluate the applicability of the updating algorithm by comparing its predictions of water table elevations obtained using MODFLOW with the HYDRUS package with the results obtained using the HYDRUS-1D and HYDRUS (2D/3D) models.

Updates of Bottom Pressure Head in the HYDRUS Package Profile to Eliminate Spurious Fluxes

Sudden inflow or outflow fluxes at the bottom of the HPM profile when the groundwater table depth changes can be eliminated if we update pressure heads at the bottom of the HPM profile at the beginning of the MODFLOW time step to an equivalent pressure head profile that would exist if there was a continuous change in the water table elevation. A pressure head profile updating algorithm was developed to achieve this objective (Fig. 1).

Figure 1 shows how the pressure head profile in the HPM profile is updated after every MODFLOW time step. Let T_1 and T_2 be two consecutive MODFLOW time steps. Initially, the average water table level (WT_1) from the MODFLOW grids is given as the bottom boundary condition (a constant bottom pressure head, h_1) to the corresponding HPM profile. The HYDRUS package simulates unsaturated flow using the 1D Richards equation until T_1. Figure 1a shows the pressure head profile in the HPM profile at time T_1.

The bottom flux q_1 calculated using this pressure head profile is given as the recharge flux to MODFLOW for simulating groundwater flow and the new water table level (WT_2) at time T_1. During the next time step, T_2, the bottom boundary condition in the HPM profile will be h_2, i.e., the pressure head corresponding to WT_2. However, imposing this pressure head boundary condition at the bottom of the HPM profile while keeping the same pressure head profile (from T_1) would produce a sudden inflow or outflow from the soil profile depending on whether the water table increased or decreased, respectively, during the time step T_1. To eliminate this sudden inflow or outflow flux, a new algorithm is proposed that adjusts pressure heads at the bottom of the HPM profile while taking into account the new groundwater table position WT_2 and the final recharge flux q_1 from the previous stress period T_1.

This can be done in a straightforward way in the saturated zone (due to the linear nature of Darcy's law), whereas a root-finding routine is used to adjust pressure heads in the unsaturated zone (due to the nonlinear nature of the Darcy–Buckingham law). According to the discretization scheme used in the HYDRUS package, the water flux between two adjacent finite element nodes i and $i+1$ in the HPM profile is expressed as

$$q=-\frac{K\left(h_i\right)+K\left(h_{i+1}\right)}{2}\left(\frac{h_{i+1}-h_i}{z_{i+1}-z_i}+1\right) \qquad [3]$$

where q is the bottom flux [L T^{-1}], K is the unsaturated hydraulic conductivity [L T^{-1}], h_i and h_{i+1} are the pressure heads in the two nodes at the bottom of the soil profile [L], and z_i and z_{i+1} are the vertical coordinates of these two nodes [L]. Equation [3] has to be solved for h_{i+1}, in which the value h_i is known and q is equal to the bottom flux. Since K depends on h_{i+1} in a strongly nonlinear manner, the equation is solved iteratively using the "false position" method (e.g., Press et al., 2007). The steady-state pressure head profile corresponding to a flux equal to q_1 and the bottom pressure head equal to h_2 is shown in Fig. 1b.

The nodal fluxes in the HPM profile at time T_1 (Fig. 1a) are then compared with the bottom recharge flux q_1, and a node is found where the relative difference is >0.1% (plus a small round-off value of 10^{-12}). The nodal pressure heads below this node are then set equal to the steady-state pressure head profile for q_1 (Fig. 1b), and the nodal pressure heads above this node are kept equal to those at T_1. This procedure is performed at every MODFLOW time step in each of the HPM profiles to eliminate sudden fluxes due to abrupt changes in the water table elevation. Figure 1c (red line) shows the pressure head profile in the HPM profile updated at the end of T_1 before moving to T_2. Note that the transition between two parts of the pressure head profile is not smooth, but it improves the consistency of the model as shown in the illustrating examples.

MODFLOW with the HPM does not represent a fully integrated modeling of flow processes in the unsaturated and saturated soil zones. Because of the stepwise change in the bottom boundary condition, calculations of a combined mass balance for both unsaturated and saturated soils are not possible. Therefore, the mass balance is considered separately for MODFLOW and the

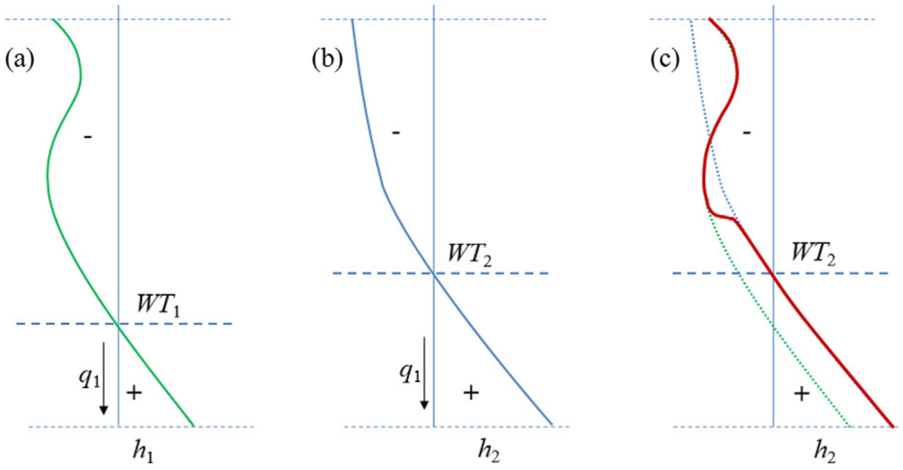

Fig. 1. Illustration of the pressure head profile updating algorithm incorporated in the HYDRUS package (HPM) to eliminate sudden variations in the bottom flux in the HPM profiles: (a) pressure head profile in the HPM profile at the end of time step T_1; (b) steady-state pressure head profile for water table level WT_2; and (c) pressure head profile in the HPM profile T_1 updated before moving to T_2 (red line).

HYDRUS package simulations. The mass balance in the original HYDRUS-1D source code is modified to account for the amount of water added or removed from the soil profile due to updating of the pressure head profile. The mass balance in the groundwater domain is calculated by including the coupling flux as the recharge to the groundwater domain (Szymkiewicz et al., 2018).

Illustrating Examples

The performance of the pressure head profile updating algorithm is illustrated using two case studies. The first case study illustrates the elimination of the sudden change in the bottom flux in the HPM profile. This case study also examines the effects of different MODFLOW time steps on the cumulative bottom flux in the HPM profile and the water table elevation obtained using MODFLOW with the HYDRUS package. The performance of the algorithm is checked by comparing the results obtained using either MODFLOW with the HPM or HYDRUS-1D.

The second case study highlights the effectiveness of MODFLOW with the HYDRUS package (which is a 3D saturated flow model coupled with a 1D unsaturated flow model) by comparing its results with HYDRUS (2D/3D) (a fully 3D model). HYDRUS (2D/3D) (Šimůnek et al., 2016) simulates water flow in both unsaturated and saturated domains by solving a three-dimensional version of the standard Richards equation. This comparison is performed to show that MODFLOW with the HYDRUS package can be used for modeling larger domains without compromising the accuracy of the results.

Case Study 1: Evaluating the Effectiveness of MODFLOW with the HYDRUS Package Using HYDRUS-1D

A domain with a length and a width both equal to 1 m and a depth of 10 m was considered in this case study. The MODFLOW domain was divided into four equal grid cells with no-flow boundaries so that the position of the water table could change only due to recharge. An atmospheric boundary condition with daily varying precipitation and potential evapotranspiration was considered at the soil surface (Fig. 2). This meteorological dataset was obtained from the weather station in Gdańsk, Poland, for 2011.

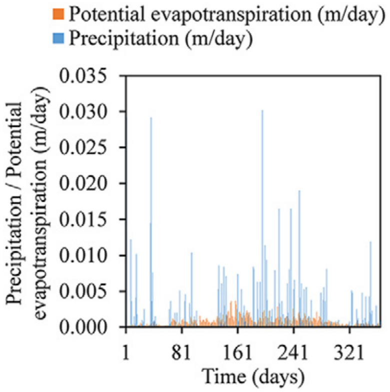

Fig. 2. Daily precipitation and potential evapotranspiration used in Case Study 1.

The HPM profiles were considered with a depth of 5 m. The soil profile was considered to have a constant pressure head equal to −0.283 m down to a depth of 3.5 m from the soil surface and a hydrostatic initial pressure head distribution below this depth. The groundwater table was considered to be initially at a depth of 3.95 m. The HPM profile was divided into 200 finite elements with relatively smaller elements near the top to ensure the convergence of the numerical solution.

The HPM profile was considered to have two soil layers: (i) a sandy soil down to a depth of 2.5 m and (ii) a loamy sand soil below this depth. The van Genuchten–Mualem analytical model (van Genuchten, 1980) was used to describe the soil hydraulic properties of the sandy and loamy sand soils. The following van Genuchten–Mualem parameters were considered for the sandy and loamy sand soils: the residual water content, $\theta_r = 0.045$ and 0.057; the saturated water content, $\theta_s = 0.43$ and 0.41; the saturated hydraulic conductivity, $K_s = 7.13$ and 3.50 m d^{-1}; the pore-connectivity parameter, $l = 0.5$ and 0.5; and the shape parameters, $\alpha = 14.5$ and 12.4 m^{-1}, and $n = 2.68$ and 2.28. The simulations were performed for 1 yr. The maximum allowed time step in the HPM simulations was 0.1 d.

The effect of different MODFLOW time steps was analyzed by dividing the duration of the simulation of 365 d into a different number of MODFLOW time steps (20, 40, and 365). In the MODFLOW domain, we assumed a constant and isotropic hydraulic conductivity equal to 3.50 m d^{-1}, the specific yield equal to 0.255, and the specific storage coefficient of 0.0015 m^{-1}.

Figure 3 shows the cumulative fluxes at the bottom of the HPM profile obtained using MODFLOW with the HYDRUS package for different numbers of MODFLOW time steps when the pressure head distribution either was or was not modified. For

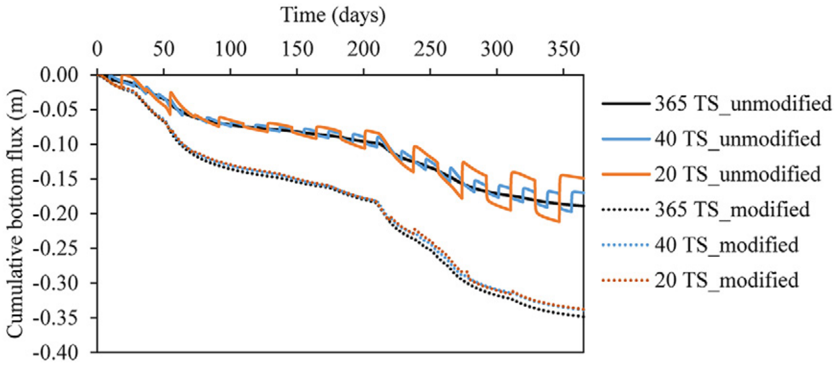

Fig. 3. Cumulative fluxes at the bottom of the HYDRUS package profile obtained using MODFLOW with the HYDRUS package for a different number of MODFLOW time steps (TS) with (modified) and without (unmodified) pressure head modifications. Negative values indicate downward flow.

all time steps, it can be observed that the cumulative bottom flux (in absolute values) increased with time. Cumulative fluxes for the simulation with the pressure head modifications were higher than when there were no pressure head modifications. This is because of the removal of upward inflow fluxes after every time step with an increase in the water table, which were generated when the pressure heads were not modified. The difference between the two sets of lines (for simulations with and without pressure head modifications) corresponds to the amount of water added to the HPM profiles as a result of the pressure head modifications.

Figure 4 shows the water table elevation obtained using MODFLOW with the HYDRUS package with and without pressure head modifications for different MODFLOW time steps. Water table elevations were found to be at a higher level when the bottom pressure head distributions were modified for all three considered MODFLOW time steps than when they were not modified. This is because of the removal of sudden upward fluxes after every MODFLOW time step, which resulted in a lower water table rise.

When the number of MODFLOW time steps is 365, the water table level is calculated by MODFLOW and provided as the bottom boundary condition to the HPM each day. When the number of MODFLOW time steps is 40 and 20, the water table elevation (the bottom boundary condition) is updated approximately only after every 9 and 18 d, respectively. As a result, the initiation of the water table rise is delayed in the latter two cases by 9 and 18 d, respectively, and the overall increase in the water table level was lower than when a smaller MODFLOW time step was used.

A constant value of the specific yield was considered in MODFLOW calculations with the HPM. The specific yield can be considered to be constant only when the aquifer response is linear, i.e., when the volume of water released is linearly proportional to the water table fluctuation. However, this is not always true because this parameter is highly dependent on the unsaturated zone properties. The specific yield determines the change in the groundwater table position in response to the simulated recharge flux and thus it determines the updated boundary condition at the bottom of each HPM profile. There have been many studies evaluating the value of the specific yield as a function of various factors that affect the specific yield, such as the transient nature of the water release from the unsaturated soil zone, soil hydraulic properties, depth of the groundwater table, or hysteresis (Nachabe, 2002; Said et al., 2005). The use of the proper value of the specific yield, taking into account unsaturated flow, is the subject of ongoing research (Stoppelenburg et al., 2005; Xu et al., 2012).

The water table elevation obtained in this case study was further compared with the results obtained using the HYDRUS-1D model by assuming a zero flux as the bottom boundary condition. The same domain and initial conditions were used in HYDRUS-1D. Figure 5 shows the comparison of the water table elevation obtained using HYDRUS-1D and MODFLOW with the HYDRUS package for different specific yield values. The temporal evolution of the water table elevation obtained with a specific yield of 0.255 was found to be the same as that obtained using HYDRUS-1D, whereas a lower value of the specific yield was found to give a larger increase in the water table elevation and vice

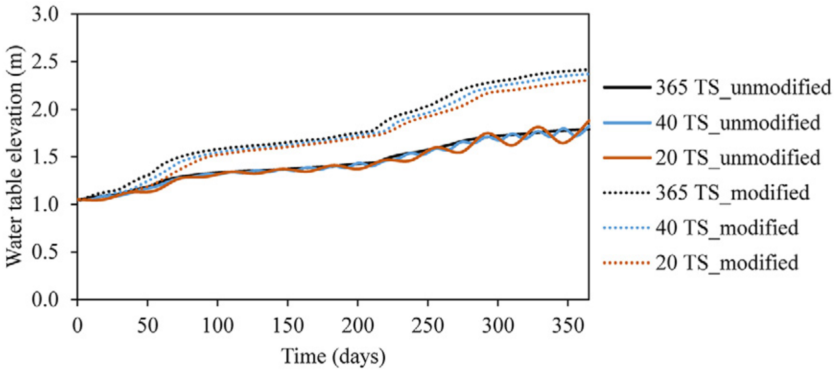

Fig. 4. Water table elevations obtained using MODFLOW with the HYDRUS package for a different number of MODFLOW time steps (TS) with (modified) and without (unmodified) pressure head modifications.

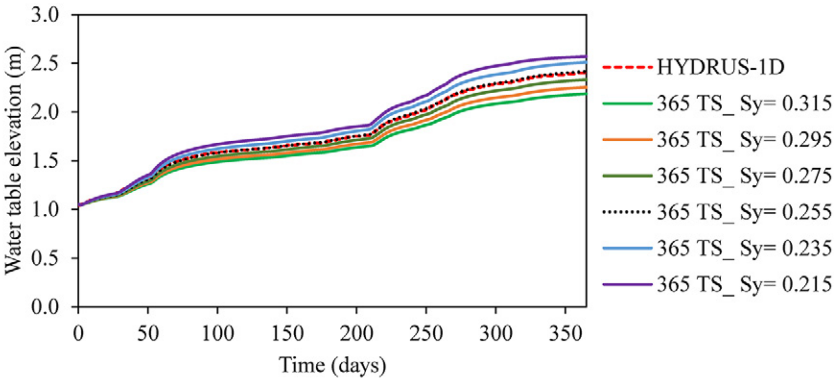

Fig. 5. The water table elevation obtained using MODFLOW with the HYDRUS package, with 365 MODFLOW time steps (TS) and different values of the specific yield (Sy), and the HYDRUS-1D model.

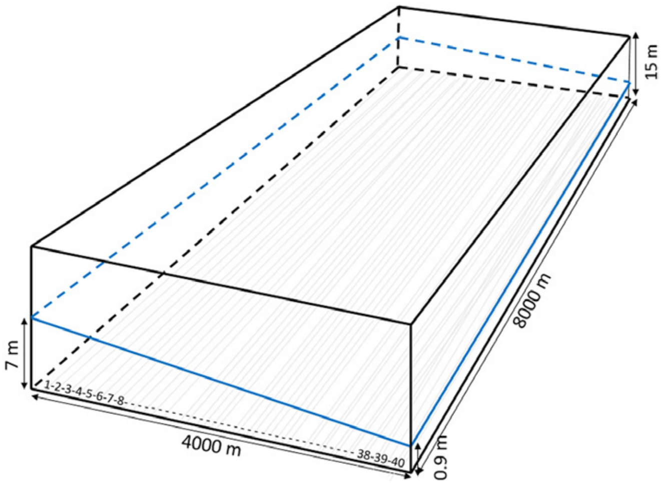

Fig. 6. Hypothetical domain and the initial water table level considered in Case Study 2.

versa. The temporal evolution of the water table elevation is highly dependent on the value of the specific yield.

Case Study 2: Evaluating the effectiveness of MODFLOW with the HYDRUS Package Using HYDRUS (2D/3D)

A hypothetical domain used in a similar study by Morway et al. (2013) was considered in this case study. The domain had dimensions of 8000 by 4000 by 15 m, with a slope of 0.001 m along the 4000-m side. The initial condition considered a groundwater table level varying between 7 m above the bottom on one side of the domain and 0.9 m on the opposite side of the domain (Fig. 6). A constant pressure head was considered along the 8000-m sides throughout the simulation. A no-flow boundary condition was assigned on the other two sides as well as at the bottom of the domain. An atmospheric boundary condition was applied at the soil surface with a monthly varying rainfall as shown in Fig. 7. The same atmospheric boundary condition was repeated during a 5-yr simulation.

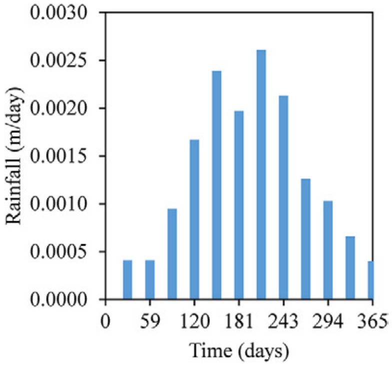

Fig. 7. Monthly precipitation considered in Case Study 2.

In MODFLOW with the HYDRUS package, the entire domain was divided into 80 rows and 40 columns (each grid had a dimension of 100 by 100 m). The MODFLOW grid cells were divided into 40 zones, and each of these zones was assigned an HPM profile (numbered from 1 to 40 in Fig. 6). The total simulation time of 1825 d was divided into 60 stress periods, with time steps equal to the number of days in the month. A specific yield of 0.28 was used.

Each HPM profile was divided into 60 finite elements of equal size. The maximum allowable time step in the HYDRUS package is 1 d. The soil was considered to be homogenous throughout the domain. The van Genuchten–Mualem analytical model (van Genuchten, 1980) was used to describe the soil hydraulic properties with the following parameters: $\theta_r = 0.1$, $\theta_s = 0.45$, $K_s = 50$ m d^{-1}, $l = 0.5$, $\alpha = 1.65$ m^{-1}, and $n = 2$. The same domain was modeled using HYDRUS (2D/3D) with the same soil hydraulic properties and with the same maximum allowable time step. Figures 8a and 8b show the initial and final pressure head distributions, respectively, in the domain obtained using HYDRUS (2D/3D).

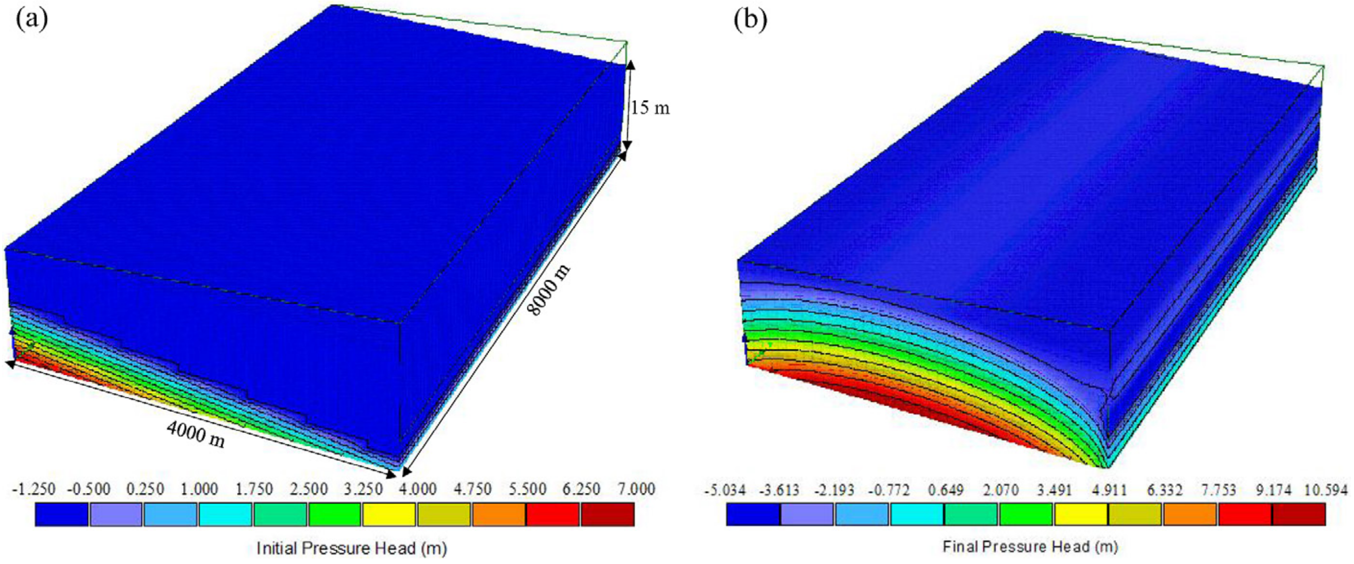

Fig. 8. (a) The initial pressure head distribution and (b) the final pressure head distribution obtained using HYDRUS (2D/3D).

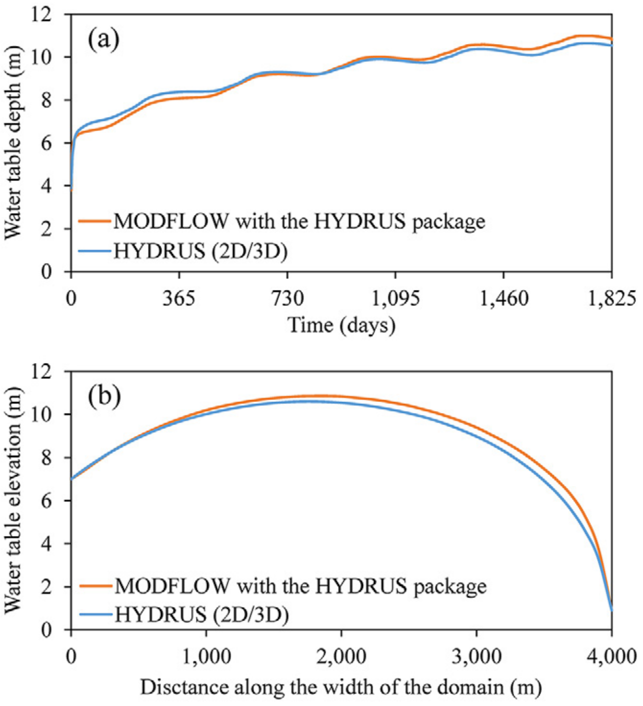

Fig. 9. Water table elevations (a) at the center of the domain and (b) at the end of the simulation along the width of the domain obtained using MODFLOW with the HYDRUS package and HYDRUS (2D/3D).

The temporal evolution of the water table elevation at the center of the domain throughout the simulation period and the final water table level along the width of the domain obtained using MODFLOW with the HYDRUS package and HYDRUS (2D/3D) are shown in Fig. 9a and 9b, respectively. The results obtained by the two models were found to be similar, which indicates that MODFLOW with the HYDRUS package is able to simulate the water table elevation accurately.

Concluding Remarks

The coupling algorithm between MODFLOW and the HYDRUS package was modified to eliminate the spurious fluxes at the HYDRUS–MODFLOW interface. The performance of the proposed method was evaluated by comparing the results obtained using MODFLOW with the HYDRUS package with the results obtained using either the HYDRUS-1D or HYDRUS (2D/3D) models. The current version of the HYDRUS package neglects the effects of unsaturated zone soil properties on the specific yield. Future research should incorporate the influence of vadose zone properties on the specific yield in the HYDRUS package, which would lead to improved modeling of water flow in the saturated–unsaturated soil zone and more accurate description of the water table dynamics.

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