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# Implementation of Solute Transport in the Vadose Zone into the

## ‘HYDRUS Package for MODFLOW’

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**Article Impact Statement:** *Solute transport is integrated into the 'HYDRUS Package for MODFLOW' and the modified model performance is evaluated using HYDRUS (2D/3D).*

## **Abstract**

The 'HYDRUS package for MODFLOW' is an existing MODFLOW package that allows MODFLOW to simultaneously evaluate transient water flow in both unsaturated and saturated zones. The package is based on incorporating parts of the HYDRUS-1D model (to simulate unsaturated water flow in the vadose zone) into MODFLOW (to simulate saturated groundwater flow). The coupled model is effective in addressing spatially-variable saturated-unsaturated hydrological processes at the regional scale. However, one of the major limitations of this coupled model is that it does not have the capability to simulate solute transport along with water flow and therefore the model cannot be employed for evaluating groundwater contamination. In this work, a modified unsaturated flow and transport package (modified HYDRUS package for

MODFLOW and MT3DMS) has been developed and linked to the three-dimensional groundwater flow model MODFLOW and the three-dimensional groundwater solute transport model MT3DMS. The new package can simulate, in addition to water flow in the vadose zone, also solute transport involving many biogeochemical processes and reactions, including first-order degradation, volatilization, linear or nonlinear sorption, one-site kinetic sorption, two-site sorption, and two-kinetic sites sorption. Due to complex interactions at the groundwater table, certain modifications of the pressure head (compared to the original coupling) and solute concentration profiles were incorporated into the modified HYDRUS package. The performance of the newly developed model is evaluated using HYDRUS (2D/3D), and the results indicate that the new model is effective in simulating the movement of water and contaminants in the saturated-unsaturated flow domains.

## **Introduction**

### **The Importance and History of Integrated Modeling**

The modeling of water flow and solute transport through saturated and unsaturated soil zones requires proper consideration of the interactions between these two zones. Accurate assessment of the movement of water and solute through these zones is important for planning and management of water resources (e.g., groundwater and surface water management, irrigation planning, groundwater pollution remediation and artificial recharge to groundwater) (Zhu et al., 2011, 2016). There are various models, from simple analytical to complex numerical, that can

independently simulate a multitude of processes in the unsaturated and saturated zones. To consider various processes and interactions in and between these zones, integrated models of varying degrees of complexity and dimensionality have been developed in the past by coupling models developed independently for unsaturated and saturated soil zones (Twarakavi et al., 2008; Ragab et al., 2010; Kalbacher et al., 2012).

The major difficulty in integrating the existing models is due to the differences in various factors that affect flow and transport in the two zones. This becomes more challenging when one has to consider the dynamic nature of the water table that is dependent on external factors such as rainfall, evapotranspiration, surface runoff, and on the soil hydraulic properties. The temporal and spatial scales of various processes in these two zones also vary. Flow in the saturated zone occurs at a slower rate and requires more time to produce significant changes in water fluxes and total heads as compared to the unsaturated zone. The spatial scale of groundwater flow applications is also significantly different (larger) than the spatial scale of the majority of vadose zone flow applications. A three-dimensional nature of flow and transport in integrated models results in increased computational time requirements along with an increased demand for model input data and physical parameters for both unsaturated and saturated zones.

Considering that flow and transport in the unsaturated zone are predominantly vertical, many integrated models have the unsaturated soil zone modeled as one dimensional along with a three-dimensional modeling of processes in the saturated zone (e.g., Niswonger et al., 2006; Twarakavi et al., 2008; Zhu et al., 2011). This simplification of the dimensionality of the problem has resulted in a significant reduction in the computational complexity. Some of the existing

integrated models are also limited to water flow and cannot consider solute transport (e.g., Niswonger et al., 2006; Twarakavi et al., 2008; Ragab et al., 2010).

Various integrated models have been developed at different levels of temporal, spatial, and dimensional complexities and with different considered processes (e.g., Refsgaard and Storm, 1995; Thoms et al., 2006; Niswonger et al., 2006; Panday et al., 2008; Twarakavi et al., 2008; Ragab et al., 2010; Brunner et al., 2012; Kalbacher et al., 2012; Morway et al., 2013). For example, MIKE SHE (Refsgaard and Storm, 1995) is a fully distributed, physically-based hydrological model that considers evapotranspiration, unsaturated flow, overland flow, groundwater flow, channel flow, and their interactions, as well as solute transport. MIKE SHE requires extensive input data and physical parameters, which makes it rather difficult to set up the model. There have been various approaches to integrating an unsaturated zone model into MODFLOW (Harbaugh et al., 2000), a widely used three-dimensional groundwater flow model, which in its basic implementation does not consider flow in the vadose zone. For example, MODFLOW-VSF (Thoms et al., 2006) models three-dimensional variably-saturated flow processes by solving the three-dimensional Richards equation. MODFLOW-UZF (Niswonger et al., 2006) uses a one-dimensional kinematic wave equation to describe flow processes in the unsaturated zone. Morway et al. (2013) used MODFLOW-UZF to first simulate variably-saturated subsurface water flow, and then, in combination with MT3DMS, also solute transport. MODFLOW-SURFACT (Panday et al., 2008) can simulate unsaturated flow and recharge, fracture flow, and contaminant transport. The HYDRUS-based flow package for MODFLOW (HPM) was developed by Seo et al. (2007) and Twarakavi et al. (2008) to simulate flow in both unsaturated and saturated zones. The package, which is based on the HYDRUS-1D model

(Šimůnek et al., 2016) simulating unsaturated water flow in the vadose zone, was linked to MODFLOW (Harbaugh et al., 2000) simulating saturated groundwater flow.

Additional examples of integrated models are IHMS (Ragab et al., 2010), HydroGeosphere (Brunner et al., 2012), and IWAS (Kalbacher et al., 2012). The Integrated Hydrological Modelling System (IHMS) developed by Ragab et al. (2010) estimates recharge from the unsaturated soil zone as a component of the water balance and provides it as input to MODFLOW. HydroGeoSphere (Brunner et al., 2012) solves three-dimensional saturated-unsaturated flow and transport equations for the vadose and saturated zones using the control volume finite element method. The IWAS toolbox (Kalbacher et al., 2012) integrates OpenGeoSys (OGS) (Kolditz et al., 2012), which solves the diffusive-wave overland flow equation and the pressure head form of the three-dimensional Richards equation, with the mesoscale Hydrologic Model (mHM) (Samaniego et al., 2011), which evaluates land surface hydrological processes, and the aRoot (Schneider et al., 2010) model, which calculates root water uptake.

### **The HYDRUS Package for MODFLOW: The Current Status**

The 'HYDRUS-based flow package for MODFLOW' (HPM) was developed by Seo et al. (2007) and Twarakavi et al. (2008) to simultaneously evaluate transient water flow in both unsaturated and saturated zones. The package, which is based on the HYDRUS-1D model (Šimůnek et al., 2016) that simulates unsaturated water flow in the vadose zone, was linked to MODFLOW (Harbaugh et al., 2000) that simulates saturated groundwater flow. Even though HYDRUS-1D

has the capability of simulating solute transport in the vadose zone, only the water flow part of HYDRUS-1D has been coupled with MODFLOW in the HPM. The HPM is effective in simulating spatially-variable saturated-unsaturated hydrological processes at the regional scale (Twarakavi et al., 2008). The HYDRUS-1D's capabilities of considering complex layering of the vadose zone and varying fluxes (both spatial and temporal) help to provide realistic input fluxes to the MODFLOW to simulate the saturated zone water flow. Applications of the HPM for regional scale groundwater flow and comparisons with the UZF1 package were described in Leterme et al. (2013, 2015). The most recent version of the HPM, which is available to the users, is compatible with MODFLOW-2005 (Harbaugh, 2005). Currently, the package is being further developed in cooperation between research groups from the University of California Riverside, the Belgian Nuclear Research Centre (SCK•CEN), and the Gdańsk University of Technology.

### **Limitations of the HPM**

The current version of the HPM can simulate water flow in unsaturated and saturated soil zones but is unable to simulate solute transport. Solute transport is highly dependent on water table fluctuations due to temporal and spatial variations in groundwater recharge. This is an important concern when the coupled model is used for analyzing groundwater contamination due to transport through the unsaturated zone.

Additionally, the current numerical coupling of HYDRUS-1D and MODFLOW produces unrealistic sudden inflow and outflow fluxes at the interface when the groundwater table depth is updated in HYDRUS-1D as a result of its change in MODFLOW (Twarakavi et al., 2009;



Kuznetsov et al., 2012). These numerical instabilities need to be resolved before the solute transport component can be incorporated into the HPM.

## Objectives

The primary objective of the study is to incorporate the solute transport into the HPM. However, to overcome the limitation of the HPM, which generated instabilities in water fluxes at the interface between the vadose and groundwater zones, was considered a priority as well, as these instabilities affect solute transport computations. The incorporation of the solute transport is achieved in two steps: (i) integrating the solute transport component of HYDRUS-1D into the HPM (hereafter referred to as ‘the modified HPM’) and (ii) coupling the modified HPM with MODFLOW and linking it with MT3DMS. The performance of the modified HPM and its coupling with MODFLOW and MT3DMS is evaluated by comparing its predictions of pressure heads, solute concentrations, and water and solute fluxes at different locations in the transport domain with the results obtained by HYDRUS (2D/3D). HYDRUS (2D/3D) (Šimůnek et al. 2016) simulates water flow and solute transport in both unsaturated and saturated domains by solving three-dimensional versions of the standard Richards and convection-dispersion equations. Finally, the dependence of time requirements of the coupled model and its particular parts (e.g., MODFLOW, the modified HPM) to spatial and temporal discretization is analyzed and discussed.

Since this manuscript frequently refers to various versions of the HYDRUS models and its modifications, as well as to the MODFLOW and MT3DMS models, the nomenclature presented in Table 1 is used to refer each model in this paper.

Table 1. Nomenclature of the models (HYDRUS and its modifications) considered in the study.

No.	Name	Description
1	MODFLOW	A modular three-dimensional groundwater flow model (Harbaugh et al., 2000).
2	MT3DMS	A modular three-dimensional multispecies solute transport model for groundwater (Zheng and Wang, 1999)
3	HYDRUS-1D	The software package for simulating the one-dimensional movement of water, heat, and multiple solutes in variably-saturated media (Šimůnek et al., 2008, 2016).
4	HYDRUS (2D/3D)	The software package for simulating the two- and three-dimensional movement of water, heat, and multiple solutes in variably-saturated media (Šimůnek et al., 2008, 2016).
5	HPM	The one-dimensional unsaturated water flow package for MODFLOW based on the HYDRUS-1D model (Seo et al., 2007; Twarakavi et al., 2008).
6	Modified HPM	A newly-developed one-dimensional unsaturated water flow and solute transport package for MODFLOW and MT3DMS

## The HYDRUS Package for MODFLOW: Modeling Approach

### Water Flow

### *Governing Equations*

Groundwater flow is modeled in MODFLOW by solving the mass conservation equation using the finite difference approximation. While MODFLOW is capable of simulating 3D flow in confined and unconfined aquifers, here we limit our analysis (without the loss of generality) to a single unconfined aquifer, represented by one layer of grid blocks. 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 follows:

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

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

HYDRUS-1D solves water flow in the unsaturated zone using the modified one-dimensional Richards equation:

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

where  $\theta$  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 the sink term [ $\text{T}^{-1}$ ], and  $K(h)$  is the unsaturated hydraulic conductivity [ $\text{LT}^{-1}$ ]. 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. HYDRUS 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 Císlerová, 1988; Kosugi, 1996; and Durner, 1994).

### *Numerical Implementation*

In MODFLOW, the groundwater modeling domain is discretized into regular grids. These grids can be combined into multiple zones based on similarities in soil hydrology, topographical characteristics, and the depth to the groundwater. In the HPM, each of these zones is assigned one soil 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 (hereafter referred to as ‘HPM profile’). Each of the HPM profiles is divided into finite elements. The soil profile can have an arbitrary number of soil layers with different soil hydraulic properties. The user can specify the number and position of nodes used to discretize each HPM profile. In order to ensure the numerical stability and efficiency, the size of finite elements should be small at locations where sharp pressure head gradients are expected, especially close to the soil surface. The details of the numerical scheme used to solve the Richards equation in HYDRUS-1D (on which the HPM is based) can be found in Šimůnek et al. (2013).

In MODFLOW, the total simulation period is divided into stress periods during which the external stresses are constant. Each stress period is divided into time steps. For each MODFLOW time step, a simulation of flow in the unsaturated zone is performed by the HPM for each HPM profile. The HPM uses its own time stepping algorithm, based on user-defined criteria. In general, HPM time steps are smaller than MODFLOW time steps because flow conditions in the vadose

zone vary more rapidly than in the saturated zone and because of the requirements of the numerical solution of the nonlinear Richards equation. 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 for the next MODFLOW time step. If a specific HPM profile is associated with more than one MODFLOW grid cell, the average value of the water table position is taken. The bottom boundary condition thus changes stepwise in the HPM. Refer to Seo et al. (2007) for more details.

#### *Updates of Pressure Heads to Eliminate Spurious Fluxes*

As discussed above, the pressure head bottom boundary condition changes in the HPM profile stepwise at the end of each MODFLOW time step. A sudden change in the position of the water table at the HPM-MODFLOW interface (i.e., the groundwater table) after every time step, and thus a change in the value of the bottom boundary condition (a time-variable pressure head boundary condition) of the HPM profile, led to either a sudden inflow into (a higher water table) or outflow from (a lower water table) the soil profile and to an incorrect cumulative bottom flux over the duration of the simulation (Twarakavi et al., 2009; Kuznetsov et al., 2012). This sudden change in the water flux when the position of the water table shifted was eliminated in the updated code by adjusting the pressure head distribution in each HPM profile after every MODFLOW time step as described below.

The updated water table level in each region at the end of the time step is obtained by the MODFLOW simulation and is then considered as the bottom boundary condition during the new time step in the HPM. The bottom pressure head in each HPM profile is set according to the new water table depth, and the pressure heads above the soil profile bottom are adjusted so that they correspond to the bottom flux at the previous time step. While this adjustment is straightforward in the saturated zone (due to a linear nature of Darcy's law), a root-finding routine was used to adjust pressure heads in the unsaturated zone (due to a non-linear nature of the Darcy-Buckingham law). According to the discretization scheme used by HYDRUS-1D and the HPM, the water flux between two adjacent nodes " $i$ " and " $i+1$ " can be expressed as:

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

The above equation has to be solved for  $h_{i+1}$ , while 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.

The steady-state nodal fluxes in the adjusted pressure head profile are compared with the nodal fluxes obtained at the end of the previous time step. The node, in which the relative difference between these two fluxes is larger than 0.1% of the flux (plus a small round off value of  $10^{-12}$ ), is set as the uppermost node, in which the pressure head profile is updated. The pressure head values below this node are set equal to the pressure heads obtained by the steady-state profile calculations for a given flux and a given position of the water table. The pressure head values above this node remain the same as the pressure heads at the end of the previous time step. This

procedure is followed after every MODFLOW time step in each HPM profile to eliminate sudden fluxes due to abrupt changes in the water table elevation.

### *Example Illustrating the Effects of the Pressure Head Updates*

The impact of updating (or not) the pressure head values at the bottom of the HPM profiles when the position of the groundwater table changes is illustrated in the following example. A domain with a length and a width both equal to 0.75 m and a depth of 10 m was considered. The MODFLOW domain was divided into nine equal grid cells (3 rows and 3 columns) with no flow boundaries so that the position of the water table could change only due to recharge. A constant inflow of  $0.002 \text{ m day}^{-1}$  was applied at the soil surface for a duration of 600 days. The soil profile was considered to have a hydrostatic initial pressure head distribution with a water table at a 5-m depth. The duration of the simulation of 600 days was divided into six equal MODFLOW time steps. The HPM column was divided into 100 finite elements of equal dimensions. The maximum considered allowable time step in HPM simulations was 0.1 day.

The van Genuchten-Mualem analytical model (van Genuchten, 1980) was used to describe the soil hydraulic properties with the following parameters: the residual water content,  $\theta_r = 0.01$ , the saturated water content,  $\theta_s = 0.3$ , the saturated hydraulic conductivity,  $K_s = 8.4 \text{ m day}^{-1}$ , the pore-connectivity parameter,  $l = 0.5$ , and the shape parameters,  $\alpha = 3.3 \text{ m}^{-1}$  and  $n = 4.1$ . The specific yield was set equal to 0.29 and the specific storage to  $0.0015 \text{ m}^{-1}$ . Note that the value of the specific yield in MODFLOW is defined independently from the soil hydraulic functions used in

the HPM. While in principle, one could use the vadose zone flow simulations to improve specific yield estimations, no such attempt was undertaken in this study.

In the HPM, the water table level obtained from MODFLOW after every time step was considered as the bottom boundary condition for the vadose zone profile simulations. The change in the water table level after every MODFLOW time step is shown in Figure 1a. Figure 1b shows the water flux at the bottom of the HPM profile when the pressure heads were not modified. The bottom flux was zero during approximately the first 45 days of the simulation, reflecting the initial hydrostatic boundary condition. A close up of the Figure 1b up to 90 days is shown in Figure 1c. Once the moisture front reached the groundwater table, the bottom flux equilibrated with the surface flux of  $0.002 \text{ m day}^{-1}$ . However, the bottom flux displayed a sudden increase (Fig. 1b) after every MODFLOW time step because of the sudden change in the bottom pressure head boundary condition in the HPM profiles, reflecting the water table levels calculated by MODFLOW. This sudden change in the bottom flux can be eliminated by adjusting the pressure head profile after every time step using the method described above. Figure 2a shows the flux at the bottom of the HPM profile when the pressure head profile was modified after each MODFLOW time step. The bottom flux was still initially zero for about 45 days, but then it increased to  $0.002 \text{ m day}^{-1}$  and remained constant at that level during the rest of the simulation. The spurious fluxes that occurred when the bottom boundary condition was changed were fully eliminated by modifying the pressure head profile using the method described above. Note that upward fluxes are positive and downward fluxes are negative in HYDRUS-1D and HPM.



Figure 2b shows the cumulative bottom flux when the pressure head distribution either was or was not modified after each MODFLOW time step. While the cumulative flux for the case with the pressure head modifications was a smooth line corresponding to the applied surface flux of  $0.002 \text{ m day}^{-1}$ , the cumulative flux for the case without the pressure head modifications exhibited sudden jumps corresponding to sudden influxes when the bottom pressure head was changed. Overall, this line has a smaller average slope than the line corresponding to the applied surface flux and is thus incorrect. The cumulative flux for the simulation with the pressure head modifications was larger than when there were no pressure head modifications (Fig. 2b). This is because of the removal of the sudden upward fluxes after every time step with an increase in the water table, which is generated when the pressure head distribution is not modified. Figure 1a shows the water table level with and without pressure head modifications. The water table level was found to be higher when the pressure head profile was modified compared to when it was not, which was also because of the removal of upward inflow after every time step.

The initial and final water content profiles for the simulation with the pressure head modification are shown in Figure 2c. The total inflow is 1.20 m, the total outflow is 1.11 m, and the change in storage is equal to 0.09 m. The mass balance was considered separately for MODFLOW and HYDRUS-1D simulations in the HPM. The mass balance calculation in the original HYDRUS-1D source code was 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).

In order to test the effectiveness of the updated coupling algorithm in the case of a falling water table, a case study similar to the one above, but considering a pumping rate of  $0.002 \text{ m}^3/\text{day}$  in the middle of the domain, was performed. This case study considered the same discretization and initial conditions as before.

The cumulative bottom flux for the case with the pressure head modifications was a smooth line while sudden jumps were observed (corresponding to sudden outflow fluxes when the bottom pressure head was changed) when the pressure head profile was not updated. The cumulative flux for the simulation with the pressure head modifications was smaller than when there were no pressure head modifications (Fig. 3b). This is because of the removal of sudden downward fluxes after every time step with a decrease in the water table, which is generated when the pressure head distribution is not modified. A corresponding change in the water table level can also be observed when the pressure head profile is not modified. Water table elevations (Figure 3a) and cumulative bottom fluxes (Figure 3b) show the effectiveness of the implementation of the new coupling algorithm.

### *The Effects of Time Steps on the Cumulative Bottom Flux*

The method discussed above for eliminating sudden fluxes at the bottom of the HPM profile when the position of the water table changes at the HYDRUS-MODFLOW interface was further tested for its functionality for different MODFLOW time steps. This was done using two case studies. Case studies 1 and 2 consider a constant and variable recharge at the soil surface, respectively.

*Case study 1: Constant Recharge*

The same domain, the same discretization, and the same initial and boundary conditions as used above were considered again. The effect of the time step on the cumulative bottom flux and the water table elevation was studied by considering three different numbers of MODFLOW time steps: 6, 60, and 600.

Figure 4a shows the cumulative bottom flux when the pressure head profile in the HPM either was or was not modified for different MODFLOW time steps. While the cumulative flux for all three cases with the pressure head modifications was a smooth line corresponding to the applied surface flux of  $0.002 \text{ m day}^{-1}$ , the cumulative flux for the cases without the pressure head modifications exhibited sudden jumps corresponding to sudden influxes when the bottom pressure head was changed. Overall, these lines have a smaller average slope than the line corresponding to the applied surface flux and are thus incorrect. Cumulative fluxes for simulations with the pressure head modifications were larger (in absolute values) compared to those without the pressure head modifications for all time steps. This is because of the removal of upward inflow fluxes after every time step with an increase in the water table which was generated when the pressure heads were not modified.

Figure 4b shows the water table elevation when the pressure head distributions either were or were not modified for different MODFLOW time steps. Water table elevations were higher when the pressure head distribution was modified for all three time steps, compared to when it was not.

This is because of the removal of the sudden upward flux after every time step, which resulted in a lower water table rise. The water table started rising after about 45 days. Simulations with 60 and 600 time steps predicted the initiation of the water table rise after approximately the same time. In the case of 6 time steps, the water table elevation (the bottom boundary condition) in MODFLOW remained constant for 100 days, which created the delayed increase in the elevation of the water table level.

This indicates the importance of choosing optimal time steps within each MODFLOW stress period in order to describe the water table dynamics accurately. Guidelines for choosing the time step in case of a transient simulation is explained in Reilly and Harbaugh (2004) and Harbaugh et al. (2000).

#### *Case study 2: Variable Recharge*

The same domain as in previous examples was used in this example as well. The length and width were both equal to 0.75 m and a depth of 10 m was considered. The MODFLOW domain was defined as such so that the position of the water table could change only due to recharge. Daily values of precipitation and potential evapotranspiration were considered for a duration of 365 days (Fig.5). The data were obtained from the weather station at the Gdańsk University of Technology, Poland, and correspond to the year 2015. The potential evapotranspiration values were divided into the potential evaporation and transpiration values using the leaf area index, which was considered to follow a typical winter wheat growth function during the entire growth period. Root water uptake for the winter wheat crop was considered using the Feddes water

uptake reduction model (Feddes et al., 1978). The following values were used for the stress response function: the pressure head below which roots start extracting water from the soil,  $P_0=0$  m, the pressure head below which roots extract water at the maximum possible rate,  $P_{Opt}=-0.005$  m, the limiting pressure head below which roots cannot extract water at the maximum rate,  $P_2=-3.0$  m, and the pressure head below which root water uptake ceases,  $P_3=-5.0$  m. Root water uptake was considered to be linearly decreasing from the soil surface to a depth of 1 m. Hysteresis in the soil hydraulic functions was not considered in this study.

The HPM profile had a depth of 5 m and a constant initial pressure head of -0.283 m down to a depth of 3.5 m and a hydrostatic equilibrium below this depth. The HPM profile was divided into 201 finite elements. Relatively small finite elements (the top element was 0.05 cm) were used at the top of the column. This is done to ensure convergence of the numerical solution and proper estimation of evaporation fluxes since the meteorological factors are expected to cause rapid changes in water content and pressure head gradients near the surface.

Two soil layers were considered: a sandy soil down to a depth of 2.5 m from the surface and loamy sand below this depth. The van Genuchten-Mualem analytical model (van Genuchten, 1980) was used to describe the soil hydraulic properties with the following parameters: the residual water content,  $\theta_r = 0.045$  (0.057), the saturated water content,  $\theta_s = 0.43$  (0.41), the saturated hydraulic conductivity,  $K_s = 7.128$  m day<sup>-1</sup> (3.502 m day<sup>-1</sup>), the pore-connectivity parameter,  $l = 0.5$  (0.5), and the shape parameters,  $\alpha = 14.5$  m<sup>-1</sup> (12.4 m<sup>-1</sup>) and  $n = 2.68$  (2.28) for the sandy soil (loamy sand). The specific yield was set to 0.353 and the specific storage to 0.0015 m<sup>-1</sup>.

Cumulative bottom fluxes and water table elevations are analyzed for different MODFLOW time steps of 10, 20, 30 and 365 days. A maximum HPM time step of 0.1 days was considered in all simulations. Figure 6a and 6b show cumulative bottom fluxes and corresponding water table elevations, respectively, obtained using the HPM for different MODFLOW time steps when the bottom pressure head distributions either were or were not modified for each considered MODFLOW time step.

Cumulative fluxes for the simulation with the pressure head modifications were higher compared to when there were no pressure head modifications (Fig. 6a). Cumulative bottom fluxes were higher for smaller MODFLOW time steps when compared to larger MODFLOW time steps.

For all considered MODFLOW time steps, water table elevations were higher when the pressure head profiles were modified compared to when they were not (Fig. 6b). This is because of the removal of the upward flux after every time step when the groundwater table rose, which resulted in a lower water table rise. As the number of MODFLOW time steps increased the water table also increased.

The relationship between modified and unmodified solutions is similar to those shown in Figure 4, when a steady infiltration rate was considered.

The method developed above to eliminate sudden inflow into (for an increasing water table) or outflow from (for a decreasing water table) the soil profile when the position of the water table

changes at the HYDRUS-MODFLOW interface has been found to be functioning well for different MODFLOW time steps and for different surface boundary conditions.

## Solute Transport

### *Governing Equations: Solute transport in the unsaturated soil zone*

The HYDRUS-1D model (Šimůnek et al., 2016) simulates solute transport in variably-saturated porous media using the standard advection-dispersion transport equation of the form:

$$\frac{\partial \theta c}{\partial t} + \rho \frac{\partial s}{\partial t} = \frac{\partial}{\partial z} \left( \theta D \frac{\partial c}{\partial z} \right) - \frac{\partial qc}{\partial z} - \phi \quad [4]$$

where  $c$  is the solution concentration [ $\text{ML}^{-3}$ ],  $s$  is the sorbed concentration [ $\text{MM}^{-1}$ ],  $D$  is the dispersion coefficient [ $\text{L}^2\text{T}^{-1}$ ],  $\rho$  is the bulk density of the porous medium [ $\text{ML}^{-3}$ ],  $q$  is the volumetric flux density [ $\text{LT}^{-1}$ ], which is obtained using the Darcy-Buckingham law, and  $\phi$  is a sink-source term accounting for various zero- and first-order or other reactions [ $\text{ML}^{-3}\text{T}^{-1}$ ] (Šimůnek and van Genuchten, 2008).

The solute transport subroutines from the standard computational module of HYDRUS-1D were integrated into the HPM to make it capable of additionally simulating the solute transport in the unsaturated zone. Once water flow is simulated in the unsaturated zone at each HYDRUS-1D time step, the nodal values of the fluid flux are determined from the nodal values of the pressure

head and the hydraulic conductivity by applying Darcy's law. The solute transport part of the code then uses these values of water contents and fluid fluxes to solve the transport equations.

Similar to HYDRUS-1D, the solute transport subroutines incorporated into the modified HPM can consider linear and nonlinear sorption, zero- and first-order production and degradation in liquid and solid phases, the one-site kinetic sorption model, the two-site sorption model with equilibrium and kinetic sorption, and the two-kinetic site sorption model (Šimůnek and van Genuchten, 2008).

#### *Governing Equations: Solute transport in the saturated soil zone*

The Modular Three-Dimensional Multispecies Transport Model (MT3DMS) (Zheng and Wang 1999) was used to simulate solute transport in the saturated soil zone. MT3DMS can simulate advection, dispersion/diffusion, and chemical reactions of contaminants in the saturated zone under general hydro-geologic conditions using the following partial differential equation:

$$\frac{\partial(\theta C)}{\partial t} = \frac{\partial}{\partial x_i} \left( \theta D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (\theta v_i C) + q_s C_s + \sum R_n \quad [5]$$

where  $C$  is the dissolved solute concentration [ $\text{ML}^{-3}$ ],  $\theta$  is the porosity of the subsurface medium (dimensionless),  $t$  is time [T],  $x_i$  is the distance along the respective Cartesian coordinate axis [L],  $D_{ij}$  is the hydrodynamic dispersion coefficient tensor [ $\text{L}^2\text{T}^{-1}$ ],  $v_i$  is the pore water velocity [ $\text{LT}^{-1}$ ],  $q_s$  is the volumetric flow rate per unit volume of the aquifer representing fluid sources (positive)



and sinks (negative)  $[T^{-1}]$ ,  $C_s$  is the concentration of the source or sink flux  $[ML^{-3}]$ , and  $\sum R_n$  is the chemical reaction term  $[ML^{-3}T^{-1}]$ .

### *Coupling Procedure*

Figure 7 shows the flowchart describing the integration of the HPM (flow and solute transport) with MODFLOW and the linking of MT3DMS with this model. The top section of the flow chart depicts the implementation of the HPM, and the bottom section depicts MODFLOW and the linking of MT3DMS, as well as their interactions at the water table. In MODFLOW, the entire simulation time is divided into stress periods, during which the external stresses are constant. These stress periods are further divided into smaller “MODFLOW” time steps. For example, in Figure 7, the total simulation period is divided into three stress periods and these stress periods are divided into two, one, and three time steps, respectively. The three-dimensional solute transport in the saturated soil zone can be further simulated using the MT3DMS package. The solution of the transport equation using MT3DMS requires much smaller time steps compared to time steps used in the MODFLOW simulation because of the stability criteria and the accuracy requirements (Zheng, 2009). For example, the MODFLOW time step 2 in the stress period 1 is divided into four smaller transport time steps (Fig.7). The HPM performs multiple time steps within each MODFLOW time step since the solution of the Richards equation requires smaller time steps compared to the time steps used by MODFLOW.

Twenty four distinct stages are required to carry out the simulation illustrated in the flow chart (Fig. 7). Initially, average water table levels from the MODFLOW grids are used as bottom

boundary conditions in the HPM profiles (stage 1). The HPM performs the water flow and solute transport simulation in the unsaturated zone for a duration of the MODFLOW time step 1 and calculates the total bottom flux and the solute concentration flux reaching the groundwater (stage 2). The total bottom flux is then given as recharge for the groundwater simulation carried out by MODFLOW (stage 3). MODFLOW solves the groundwater flow equation for time step 1 and calculates the updated water table level (stage 4). This water table level is assigned as the bottom boundary condition in the HPM (stage 5). The solute flux can be provided as the concentration flux input to MT3DMS to simulate the solute transport in the saturated soil zone.

Before moving to stage 6, the pressure head distribution at the bottom of the HPM profiles at the end of the first time step is modified to eliminate sudden fluxes using the method discussed above. This is followed by the modifications of solute concentrations corresponding to the modifications of pressure heads using the method discussed below. The HPM again solves the solute transport and water flow for a duration of MODFLOW time step 2 (stage 6). Stages 7, 11, 15, 19, and 23 perform the same task as stage 3. Stages 6, 10, 14, 18, and 22 perform tasks similar to stage 2, and stages 8, 12, 16, 20, and 24 perform steps similar to stage 4.

### *Updates of Solute Concentrations*

Since the pressure head (water content) distributions are updated after each MODFLOW time step (to eliminate the effects of sudden fluxes at the HYDRUS-MODFLOW interface and to fix the overall mass balance errors), solute concentrations need to be correspondingly adjusted to preserve the mass balance. This was done by either lowering (diluting) or increasing

(concentrating) solute concentrations, depending on the change in water contents due to the modification of the pressure heads. The new concentration was obtained by equating the total solute mass (the mass of solute per volume of soil) before and after the adjustment of the water content profile at each node where water contents were updated:

$$\left( \frac{\rho K_d c^\beta}{1 + \eta c^\beta} + \theta c \right)_{old} = \left( \frac{\rho K_d c^\beta}{1 + \eta c^\beta} + \theta c \right)_{new} \quad [6]$$

In Eq. 6,  $K_d$ ,  $\beta$ , and  $\eta$  are empirical coefficients of the adsorption isotherm that is used in HYDRUS-1D and the modified HPM,  $\theta$  is the volumetric water content,  $c_{new}$  is the updated solution concentration,  $c_{old}$  is the original solution concentration, and  $\rho$  is the bulk density of the porous medium.

For linear sorption ( $\beta=1$  and  $\eta=0$ ), the solution of Eq. 6 is trivial, and  $c_{new}$  is obtained by solving Eq. 7:

$$c_{new} = c_{old} \frac{(\rho K_d + \theta)_{old}}{(\rho K_d + \theta)_{new}} = c_{old} \frac{\rho K_d + \theta_{old}}{\rho K_d + \theta_{new}} \quad [7]$$

For nonlinear sorption (i.e., Langmuir or Freundlich,  $\eta>0$  or  $\beta \neq 1$ , respectively),  $c_{new}$  is obtained by the Brent method for finding roots of nonlinear equations (Press et al., 1992).

### ***Example Illustrating the Effects of the Concentration Updates***

The same example discussed above in Section "Example Illustrating the Effects of the Pressure Head Updates" is considered here. A solute concentration of  $5 \text{ mg l}^{-1}$  was considered along with a constant inflow of  $0.002 \text{ m day}^{-1}$ . The bulk density of the soil was assumed to be  $1.5 \text{ g cm}^{-3}$  with a longitudinal dispersivity  $0.1 \text{ m}$ . Since the entire simulation for 600 days was divided into six equal MODFLOW time steps, the concentrations after every MODFLOW time step were updated correspondingly to the modifications of the pressure heads and water contents. Figure 8 shows the change in the water content profile (corresponding to the pressure head modifications) after the fifth time step and corresponding changes in the concentration profile. The modified pressure head profile resulted in higher water contents in the soil immediately above the water table. Hence, the updating method lowers (dilutes) the solute concentration correspondingly to an increase in the water content.

### **Performance Evaluation of the Modified HPM Using HYDRUS (2D/3D)**

The performance of the newly developed modified HPM was evaluated by comparing its results with the results of the two-dimensional simulation with HYDRUS (2D/3D) (referred to below as HYDRUS-2D). Similar to HYDRUS-1D, HYDRUS-2D simulates water flow and solute transport in both unsaturated and saturated domains by solving the two-dimensional versions of the standard Richards and convection-dispersion equations (Eqs. 2 and 4, respectively).

### ***Case Study***

A hypothetical two-dimensional domain was considered for the performance evaluation of the modified HPM with HYDRUS-2D. The domain has a width of 100 m and a depth of 10 m. This

domain was considered to have 20 MODFLOW grids and 20 HPM (HP-1 through HP-20) soil profiles. The initial pressure heads in the HPM profiles were assumed to be in hydrostatic equilibrium. The initial water table in the entire domain was set at a depth varying from 4.0 to 6.0 m between the left and right sides of the domain. While four HPM profiles (HP-9, HP-10, HP-11, HP-12) were assumed to have a constant recharge of  $0.04 \text{ m day}^{-1}$  with a solute concentration of  $5 \text{ mg/l}$  at the soil surface, there was no recharge considered in the remaining HPM profiles throughout the simulation period. Such a setting represents infiltration from a pond or effluent lagoon, or artificial recharge using treated wastewater. The total simulation time was 100 days. The number of stress periods (MODFLOW time steps) was also 100, each having a time step duration of one day. A constant head of 6.0 m and 4.0 m was assumed at left and right ends of the domain respectively. Figure 9 shows the transport domain considered in our study.

The van Genuchten-Mualem analytical model was used to describe the soil hydraulic properties with the following parameters:  $\theta_r = 0.01$ ,  $\theta_s = 0.3$ ,  $K_s = 8.4 \text{ m day}^{-1}$ ,  $l = 0.5$ ,  $\alpha = 3.3 \text{ m}^{-1}$ , and  $n = 4.1$ . The specific yield was set equal to 0.29 and the specific storage to  $0.0015 \text{ m}^{-1}$ . A bulk density of  $1.5 \text{ g/cm}^3$  and a longitudinal dispersivity of 1 m was assumed. Solute transport without adsorption was considered here. Each 10 m deep HPM profile was divided into 100 finite elements of equal widths. A maximum allowable time step of 1 day was considered in the simulation.

The same domain was modeled using HYDRUS-2D. In HYDRUS-2D, the entire domain was discretized spatially into a finite element mesh, with relatively small elements at locations

where large hydraulic gradients were expected. An average value of 0.05 m was considered as the size of the finite element towards the soil surface whereas a size of 0.3 m was considered towards the bottom of the domain. The same water flow and solute transport parameters used in the modified HPM were considered along with a transverse dispersivity of 0.1 m. A maximum time step of 1 day was considered here as well.

Figure 10 shows a comparison of water table variations, solute concentrations reaching the water table, and water and solute fluxes reaching the water table calculated with the modified HPM (HPM-20 HP) and HYDRUS-2D. Figure 10a shows a comparison of water table elevations at the center of the transport domain calculated by HYDRUS-2D and the modified HPM during the simulation. An increase in the water table elevation is almost the same for both models. Similarly, solute concentrations (Fig.10c) and water and solute fluxes (Fig.10b and d) reaching the water table at the center of the domain are also comparable in both models. This comparison shows that the solute transport component incorporated into the HPM is functioning well and can simulate the solute transport in the unsaturated zone accurately.

***The Effects of Spatial Discretization on the Computational Time and Accuracy of the Results.***

A significant saving of computational time can be achieved by reducing the number of HPM profiles considered in the unsaturated soil zone if this can be achieved without compromising the accuracy of the results. The same example problem discussed in the previous section was further analyzed for the computational time requirement and the accuracy of the results by varying the number of HPM profiles. Four cases were considered in the analysis. In Case 1, the domain had 20 HPM profiles (HP-1, HP-2, HP-3, ..., up to HP-20) (Fig.9). Case 2 considered 10 HPM profiles (HP-1, HP-2, HP-3, ..., up to HP-10), Case 3 considered only 5 HPM profiles (HP-1, HP-2, HP-3, HP-4 and HP-5), and Case 4 considered only 1 HPM profile (HP-1). The HP-9, HP-10, HP-11, and HP-12 profiles in Case 1, the HP-5 and HP-6 profiles in Case 2, the HP-3 profile in Case 3, and the HP-1 profile in Case 4 were assumed to have a constant recharge of  $0.04 \text{ m day}^{-1}$  with a solute concentration of  $5 \text{ mg/l}$  at the soil surface. No recharge was considered in other HPM profiles during the entire simulation period in all three cases. In Case 4, no HPM profiles were required in the part of the domain, which did not receive any recharge.

Figure 10 shows a comparison of water table variations, solute concentrations reaching the water table, and water and solute fluxes reaching the water table in the center of the domain obtained in four scenarios analyzed by the modified HPM and HYDRUS-2D. Water table elevations, bottom fluxes, solute concentrations, and concentration fluxes simulated in all four modified HPM scenarios and by HYDRUS-2D are almost the same. In Figure 10a, the water table elevation in the center of the domain was found to be slightly lower when a smaller number of HPM profiles was considered. This is because of the averaging of the water table elevation in the MODFLOW grid cells assigned to the same HPM profiles. The averaging of the water table results in a lower level of the water table, which is given as a bottom boundary condition to the HPM profile. For

example, in Case 1, in which each MODFLOW grid was assigned one HPM profile, the water table level obtained by MODFLOW is given to the corresponding HPM profile without any averaging. In Case 2, the water table averaged after every time step for several MODFLOW grid cells (i.e., 1, 2; 3, 4; 5, 6; 7, 8; 9,10; 11, 12; 13, 14; 15, 16; 17, 18; and 19 and 20) are given as the bottom boundary condition to the HPM profiles (HP-1, HP-2, HP-3, HP-4, HP-5, HP-6, HP-7, HP-8, HP-9 and HP-10 respectively). In Case 3, the average water table in MODFLOW grid cells (1, 2, 3, 4; 5, 6, 7, 8; 9, 11, 12; 13, 14, 15, 16; and 17, 18, 19, 20) is given as the bottom boundary condition to the HP-1, HP-2, HP-3, HP-4 and HP-5 profiles, respectively. In Case 4, the average water table from MODFLOW grids (9, 10, 11, 12) is given as the bottom boundary condition to the HP-1 profile.

The total computational time (on a PC with the Intel i7 processor and the Windows 7 operating system) required in Case 1 was 17.36 seconds, whereas in Cases 2, 3, and 4 it was 9.31, 4.42, and 2.01 seconds, respectively. The total number of nodes in the HPM profiles in Case 1, Case 2, Case 3, and Case 4 were (20 profiles\*101 nodes) 2020, (10\*101) 1010, (5\*101) 505, and (1\*101)101, respectively, along with 20 MODFLOW grids. This has resulted in a significant decrease in the computational time requirement of the simulations. This shows that we can reduce the computational time of the modified HPM using a proper spatial discretization and the allocation of HPM profiles to each MODFLOW grid.

## **The Use of MT3DMS for the Saturated Zone Solute Transport Modeling**

### ***Recharge and Solute Flux from the Modified HPM as Input to MT3DMS***



The solute transport in the saturated zone is simulated using MT3DMS, which is not fully coupled with MODFLOW and the modified HPM. Since the water and solute concentration fluxes reaching the groundwater are obtained from the modified HPM, this information can be fed into MT3DMS to simulate the solute transport in the saturated soil zone. The MT3DMS code is a standalone transport simulation model, which can be used with any finite difference flow model. MT3DMS is often used in conjunction with the widely accepted groundwater flow model MODFLOW. LMT (Zheng et al., 2001) is an add-on package for MT3DMS that has been developed to save the flow solution (cell by cell heads and fluxes, and locations and flow rates from sources and sinks solved by MODFLOW) that is required for the simulation of the solute transport in the saturated soil zone. The LMT package is used for linking the results of MODFLOW with the modified HPM and MT3DMS. The solute concentration flux reaching the water table calculated by the modified HPM is provided as the concentration flux input to MT3DMS to simulate the solute transport in the saturated soil zone. Since MT3DMS is not fully integrated into the MODFLOW-HYDRUS program, the solute transport simulation can be carried out using the LMT package (Zheng et al., 2001), which allows MODFLOW to store the flow information (cell by cell heads and fluxes, and locations and flow rates from sources and sinks solved by MODFLOW) for each time step in the saturated zone, which is then further used by MT3DMS.

### *Case Study*

The case study discussed in the previous section is further analyzed in combination with MT3DMS. The solute concentration flux at the water table at each time step obtained using the modified HPM is considered as the concentration flux input for the MT3DMS simulations of the saturated soil zone. The same solute transport parameters as used in HYDRUS-2D were also used in MT3DMS. An effective porosity of 0.3 and a longitudinal dispersivity of 1m was considered. The ratio of the horizontal transverse dispersivity to the longitudinal dispersivity was assumed as 0.1, and the ratio of the vertical transverse dispersivity to the longitudinal dispersivity was assumed as 0.01.

Figure 11 shows the concentration profiles in the transport domain obtained by MT3DMS and HYDRUS-2D at the end of the simulation. Two cross sections (Fig. 11, left), one at the center of the domain (1) and one at a distance of 20 m from the center of the domain (2), were considered in the further analysis. Figure 12a and Figure 12b shows the comparison of concentrations along these two cross sections obtained using MT3DMS and HYDRUS-2D at the end of the simulation.

The solute concentration below the water table (the water table is 4.52 m below the soil surface in section 1 and 5.033 m in section 2) is comparable in both models. The concentration in the saturated zone obtained using MT3DMS is influenced by various factors such as horizontal and vertical transverse dispersivity, the spatial and temporal discretization, and the wetting factor used in MODFLOW for converting the dry cell to wet cell. The differences in the concentration profiles obtained using MT3DMS and HYDRUS-2D are mainly caused by the differences in the spatial discretization used. While rectangular grids were considered in the MT3DMS simulation, the finite element mesh in HYDRUS-2D was constructed by dividing the flow region into

quadrilateral and/or triangular elements. These discretizations are not the same due to different solution techniques and convergence criteria used in both models.

### **Computational Time Requirements of the Coupled Model and its Components.**

The computational efficiency of the developed model was analyzed by comparing the total computational time used by (i) MODFLOW with the modified HPM, (ii) the modified HPM itself, and (iii) the HYDRUS-2D model using the case study discussed above.

The total simulation time was 100 days. The computer used for running the model was Intel i7 processor with Windows 7 operating system. When the number of considered time steps was 100 (with each MODFLOW time step duration of one day), the total computational time required for MODFLOW with the modified HPM was 17.36 s, from which the modified HPM required 14.95 s. This shows that most computational time required by the model was used for simulating processes in the unsaturated zone. This is because of the increased computational time requirements for the numerical solution of the Richards equation for simulating water flow in the unsaturated soil zone when compared to the solution of the groundwater flow equation for the saturated soil zone. Note that in this case study, the total number of nodes in the HPM profiles in the unsaturated zone was 2020 (20 profiles \* 101 nodes), whereas the saturated zone had only 20 MODFLOW cells, which well explains the higher computational time requirement of the modified HPM.

When the same case study was solved using HYDRUS-2D (with a maximum allowable time step of one day), the computational time was 295.14 s. HYDRUS-2D required more computational time when compared to MODFLOW with the modified HPM.

Table 2. Computational time of the entire MODFLOW model with the modified HPM and the vadose zone simulations in the modified HPM for different MODFLOW time steps.

No. of MODFLOW time steps	Computational time (Seconds)	
	The modified HPM	MODFLOW with the modified HPM
5	4.92	5.67
10	5.12	5.89
20	5.53	6.52
40	6.52	7.82
60	9.15	11.10
80	12.80	14.98
100	14.95	17.36

The total computational time of the MODFLOW model coupled with the modified HPM and the HPM depends on the number of MODFLOW time steps (Table 2). In this study, the total simulation time is divided into MODFLOW time steps of equal duration. The computational time of MODFLOW with the modified HPM is found to be increasing with an increase in the number of time steps. It can also be observed that the vadose zone simulation time in the modified HPM constitutes a major percentage of the total computational time for different time steps.

It can also be observed in Table 2 that the overall computational time, and especially the modified HPM computation time, is increasing only slowly when there are fewer MODFLOW time steps (5, 10, 20, 40). However, with a further increase in the number of MODFLOW time steps, the computational time starts increasing exponentially. This is likely due to temporal discretization criteria used in the HPM. The number of time steps in the modified HPM is almost the same when the number of the MODFLOW time steps is small (less than 40 in this case) and larger MODFLOW time steps have only a limited impact on HPM time steps. However, when the number of MODFLOW time steps is large, i.e., MODFLOW time steps are small, the HPM is required to take smaller time steps as well and their number increases. More information on the time step control can be found in Šimůnek et al. (2013).

## Summary and Conclusions

The major limitation of the HPM was that it generated instabilities in water fluxes at the saturated-unsaturated interface when the position of the water table changed. This limitation is addressed by updating the coupling algorithm. The new algorithm has been tested on a large number of examples and found to be functioning well for different MODFLOW time steps. The modified HPM does not create spurious fluxes at the bottom of the soil profiles for any temporal discretization used in MODFLOW.

Since the original HPM did not have the capabilities of simulating solute transport, the HPM was modified by incorporating the solute transport component of HYDRUS-1D and linking it with

MT3DMS. The linking of the HPM with MT3DMS requires additional processing of information from MODFLOW and the HPM before MT3DMS can be run.

The performance of the entire modeling system involving MODFLOW, the modified HPM, and MT3DMS, proposed in this study, was evaluated by comparing its predictions of pressure heads, solute concentrations, and water and solute fluxes at different locations in the transport domain with the results obtained using HYDRUS (2D/3D). Since the simulation results were in close agreement, the proposed modeling system can be used to comprehensively simulate water flow and solute transport processes in the saturated-unsaturated zones. The future research can focus on tighter coupling of MODFLOW with the modified HPM and MT3DMS so that user interventions can be fully eliminated. The analysis of computational time requirements of MODFLOW with the modified HPM shows that most CPU time is used by the HPM to simulate processes in the unsaturated zone and only a small fraction of time is used by MODFLOW itself. Therefore, by choosing appropriate MODFLOW time steps and spatial discretizations, one can achieve a considerable reduction in the computational time requirement.

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Figure 1. Water table elevations with and without pressure head modifications at each MODFLOW time step (a), the flux at the bottom of the HPM profile without pressure head modifications (b) and the close-up view of the cumulative bottom flux up to 90 days (c).

Figure 2. The flux at the bottom of the HPM profile for the simulation with the pressure head modifications (a), cumulative fluxes at the bottom of the HPM profile for simulations with and without pressure head modifications (b), and the initial and final water content profiles for the simulation with the pressure head modification (c).

Figure 3. Water table elevations (a) and cumulative bottom fluxes (b) in the HPM profile with and without pressure head modifications after each MODFLOW time step.

Figure 4. Cumulative fluxes at the bottom of the HPM profile (a) and water table elevations (b) obtained using the HPM for different MODFLOW time steps (TS) with and without pressure head modifications.

Figure 5. Daily precipitation and potential evapotranspiration for the variable recharge case study.

Figure 6. Cumulative fluxes at the bottom of the HPM profile (a) and water table elevations (b) obtained using the HPM for different MODFLOW time steps (TS) with and without pressure head modifications.

Figure 7. Flowchart describing the integration of the modified HPM (including solute transport component) into MODFLOW.

Figure 8. The original and updated water contents and solute concentrations in response to the modification of the pressure heads (before\* and after\* refers to before and after the pressure head profile updating).

Figure 9. A schematic showing the flow and transport domain. Cases 1, 2, 3, and 4 indicate evaluated scenarios with different numbers of considered HPM profiles.

Figure 10. Water table elevations (a), water fluxes (b), solute concentrations (c), and solute fluxes (d) at the water table in the center of the domain obtained using HYDRUS-2D and the modified HPM with different numbers of profiles.

Figure 11. Concentration profiles in the transport domain at the end of the simulation obtained using MT3DMS (left) and HYDRUS-2D (right). Two vertical profiles (1 and 2) in the left figure are used in Figure 12.

Figure 12. A comparison of solute concentrations in the saturated zone obtained by MT3DMS and HYDRUS-2D on vertical profiles defined in Figure 11.





















































