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A Comprehensive Quasi-3D Model for Regional-Scale Unsaturated-Saturated Water Flow

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Abstract: For computationally efficient modeling of unsaturated-saturated flow systems of regional scale, it is necessary to use Quasi three-dimensional (3-D) schemes that consider one-dimensional (1-D) soil water flow and 3-D groundwater flow. However, it is still practically challenging for regional-scale problems due to the high non-linear and intensive input data needed for soil water modeling, the reliability of the coupling scheme, and the complicated modeling operation. This study developed a new Quasi-3D model coupled the soil water balance model UBMOD with MODFLOW. A new iterative scheme was developed, in which the vertical net recharge and unsaturated zone depth were used as the exchange information. A modeling framework was developed by Python script to wrap the coupled model, the pre- and the post-process modules, which gave a comprehensive modeling tool from data preparation to results displaying. The strength and weakness of the coupled model are evaluated by using two published studies. The comparison results show that the coupled model is satisfactory in terms of computational accuracy, mass balance error and cost. Additionally, the coupled model is used to evaluate groundwater recharge in a real-world study. The measured groundwater table and soil water content are used to calibrate the model parameters, and the groundwater recharge data from a two years' tracer experiment is used to evaluate the recharge estimation. The field application further shows the practicability of the model. The developed model and the modeling framework provide a convenient and flexible tool for evaluating unsaturated-saturated flow system at the regional scale.

1 Introduction

While groundwater resource is important for the domestic, agricultural, and industrial uses, groundwater is vulnerable due to over-exploitation, climate change, and biochemical pollution (Bouwer, 2000; Sophocleous, 2005; Evans and Sadler, 2008;

Karandish et al., 2015; Zhang et al., 2018). For protecting or exploiting groundwater resource, understanding soil water flow system is necessary as soil water is the major source of groundwater recharge and destination of phreatic consumption (Yang et al., 2016; Wang et al., 2017). The extended form of the Richards' equation is usually used to describe the soil water flow and groundwater flow. Many numerical schemes have been developed to solve the three-dimensional (3-D) Richards' equation (Weill et al., 2009) in computer codes, such as HYDRUS (Šimůnek et al., 2012), FEFLOW (Diersch, 2013), HydroGeoSpere (Brunner and Simmons, 2012), InHM (VanderKwaak and Loague, 2001) and MODHMS (Tian et al., 2015). Since the soil water flow is highly nonlinear in nature and sensitive to atmospheric changes, soil utilizations, and human activities, the numerical schemes require using fine discretization in space and time for accurate numerical solutions (Downer and Ogden, 2004; Varado et al., 2006). This makes the numerical solutions computationally expensive, especially for large scale modeling; the fine discretization also leads to a mismatch with saturated groundwater flow, because the latter solutions are commonly based on coarse discretization. (Van Walsum and Groenendijk, 2008; Shen and Phanikumar, 2010; Yang et al., 2016; Szymkiewicz et al., 2018).

To address the computational challenges discussed above, a variety of simplifications have been introduced for the soil water flow for regional scale problems. One simplification is to treat the hydrological processes (e.g., infiltration, evapotranspiration, and deep percolation) occurring in the unsaturated zone as one-dimensional (1-D) processes in the vertical direction. Field experiments at the regional scale also show that, in the unsaturated zone, the lateral hydraulic gradient is usually significantly smaller than the vertical gradient (Sherlock et al., 2002). This 1-D simplification leads to the Quasi-3D scheme, which ignores the lateral flow in the unsaturated zone but considers groundwater flow as a 3-D problem. The Quasi-3D scheme avoids solving the 3-D Richards' equation for the unsaturated zone, and thus improves computational efficiency and model stability. The Quasi-3D scheme is the most efficient solution for large-scale unsaturated-saturated flow modeling (Twarakavi, et al., 2008; Yang et al., 2016) and is popular among groundwater modelers (Havard et al., 1995; Harter and Hopmans, 2004; Graham and Butts, 2005; Stoppelenburg et al., 2005; Seo et al., 2007; Markstrom et al., 2008; Ranatunga et al., 2008; Kuznetsov et al., 2012; Xu et al., 2012; Zhu et al., 2012; Maxwell et al., 2014; Leterme et al., 2015). However, it is still challenging when using the Quasi-3D models for a practical regional scale problem. Three concerns arise as follows.

The first concern is the unsaturated modeling method. Although the Quasi-3D scheme is computationally efficient, the numerical solutions of the 1-D Richards' equation still require intensive input data, and face numerical instability and mass balance errors under some specific situations such as infiltration into the dry soil (Zha et al., 2017), which limit their practical application to simulating regional scale problems under complicated geological and climate conditions as well as anthropogenic activities. As an alternative to the numerical solutions of the 1-D Richards' equation,

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water balance models have been used to describe soil water movements, which not only reduces the amount of input data but also further improve computational efficiency and stability for simulating soil water movement. The water balance models can be coupled with groundwater models. Facchi et al. (2004) coupled a conceptual soil water movement model SVAT with MODFLOW to simulate the hydrological relevant processes in the alluvial irrigated plains. Kim et al. (2008) integrated SWAT with MODFLOW to describe the exchange between hydrologic response units in the SWAT model and MODFLOW cells. The traditional water balance models however, may oversimplify soil water movement, and thus cannot accurately represent certain important features of soil water flow, e.g., the upward flux and soil heterogeneity. Mao et al. (2018) developed a soil water balance model (called UBMOD model) based on the hybrid of numerical and statistical methods. In particular, UBMOD can simulate both upward and downward soil water movement in heterogeneous situation with only four model parameters, and the model can be used with a coarse discretization in space and time, all of which make it suitable for the large-scale modeling.

Another concern is the scheme when coupling saturated models with unsaturated models. There are three different numerical coupling schemes categorized by Furman (2008): uncoupled, iterative coupled, and fully coupled. The uncoupled scheme is widely used when using soil water flow packages with MODFLOW, such as LINKFLOW (Havard et al., 1995), SVAT-MODFLOW (Facchi et al., 2004), UZF1-MODFLOW (Niswonger et al., 2006), HYDRUS-MODFLOW (Seo et al., 2007), SWAP-MODFLOW (Xu et al., 2012). While this scheme is easy to be implemented, its results may not reliable when recharge from the unsaturated zone causes substantial changes of water table. Additionally, this scheme may result in the mass balance error (Shen and Phanikumar, 2010; Kuznetsov et al., 2012). The fully coupled scheme is mathematically and computationally rigorous, because it solves unsaturated and saturated flows simultaneously with internal boundary conditions of the two flows (Zhu et al., 2012). However, the fully coupled scheme is computationally expensive (Furman, 2008). The iterative coupled scheme offers a trade-off between model accuracy and computational cost (Yakirevich et al., 1998; Liang et al., 2003), and has been used to couple two hydrodynamic models with the hydraulic head of the internal boundary being used as the exchange information (Stoppelenburg et al., 2005; Kuznetsov et al., 2012). However, the soil water content is the variable used by soil water balance models other than the hydraulic head. Therefore, a specific iterative scheme should be developed to couple the soil water balance model using the water content and the hydrodynamic groundwater model using the hydraulic head.

The third concern is about practicability. Many Quasi-3D models are focus on the algorithms, while lacking the pre- and post-processing tools for handling the spatial information, which limit the model application for a practical regional scale problem with complicated hydrogeological properties and boundary conditions (Zhu et al., 2013).

In this study, a new Quasi-3D model is developed. The 1-D water balance model

UBMOD developed by Mao et al. (2018) is integrated with MODFLOW (Harbaugh, 2005). A new iterative scheme is established for numerical solutions, and the net groundwater recharge and the depth of unsaturated zone are chosen as the exchange information. The coupling model can achieve mass balance and keep numerical stability well, and the model is suitable for large-scale modeling based on the characteristics of MODFLOW and UBMOD. Moreover, instead of developing a new package for MODFLOW, a framework of organizing the modeling procedures by Python scripts is developed, which wraps the coupled model, pre- and post-processing tools. The framework embeds a powerful function of geographic information processing with the help of Python packages for data preparation and results displaying, thus makes the modeling tool convenient and flexible for practical uses. This paper elaborates the methodology of coupling the unsaturated and saturated water flow and the modeling framework in Sect. 2. Two published studies are used to test the performance of the coupled model when handling different water flow conditions in Sect. 3. A real-world application to study the regional net groundwater recharge is presented in Sect. 4.

2 Methodology and Model Development

In the new coupled model, the unsaturated-saturated domain is partitioned into a number of sub-areas in the horizontal direction mainly according to the spatially distributed inputs (soil types, atmosphere boundary conditions, land uses, and crop types). A 1-D soil column is used to characterize the average soil water flow in each

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sub-area, and UBMOD is used to simulate the 1-D soil water flow. MODFLOW is used to simulate the 3-D groundwater flow of the whole model domain. It assumed that the flow in the unsaturated zone is in the vertical direction, and that there is only vertical exchange flux between the unsaturated and saturated zones. It is further assumed that using the vertical column can reasonably simulate the unsaturated flow in each sub-area while ignoring the horizontal heterogeneity. In this section, UBMOD is first presented, followed by a brief introduction of MODFLOW and two peripheral tools (FloPy (Bakker et al., 2016) and ArcPy (Toms, 2015) used in the new model. The procedures of the new model and the modeling framework are described in Sect. 2.3 and the specific unsaturated and saturated coupling scheme is described in Sect. 2.4.

2.1 The Soil Water Balance Model UBMOD

This section briefly describes the soil water balance model UBMOD to make this paper self-contained, and more details of UBMOD are referred to Mao et al. (2018). Before the calculation, the domain is discretized into a series of soil layers, and the simulation period is discretized into time steps. UBMOD has four major components to describe the soil water movement in a given time step. The first one is the allocation of the infiltration water if there is precipitation or irrigation on ground surface, and the other three components correspond to the three forces (the gravitational potential, source/sink term for external forces and the matric potential) driving the soil water movement. The governing equations of the model are as follows,

$$q = \min\left(M \times (\theta_s - \theta), I - I_d\right), \tag{1}$$

for the amount of allocated infiltration water of a given layer,

$$\frac{\partial \theta}{\partial t} = -\frac{\partial K(\theta)}{\partial z}, \tag{2}$$

for the advective movement driven by the gravitational potential,

$$\frac{\partial \theta}{\partial t} = -W, \tag{3}$$

for source/sink terms, and

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(D(\theta)\frac{\partial \theta}{\partial z}\right), \tag{4}$$

for diffusive movement driven by the matric potential. In these equations, q is the amount of allocated water per unit area of the layer [L]; M is the thickness of each soil layer [L]; θ is the soil water content [L^3L^{-3}]; θ_s is the saturated soil water content [L^3L^{-3}]; I is the quantity of infiltration water per unit area [L]; I_d is the allocated amount of infiltration water per unit area specified before the calculation [L]; t is the time [T]; $K(\theta)$ is the unsaturated hydraulic conductivity [LT^{-1}] as a function of soil water content; z is the elevation in the vertical direction [L]; W is the source/sink term [T^{-1}] to account for soil evaporation and root uptake term of crop transpiration; $D(\theta)$ is the hydraulic diffusivity [L^2T^{-1}], $D(\theta) = K(\theta) \times \partial h / \partial \theta$, where h is the pressure head [L].

The equations are solved in sequence in the UBMOD. The unsaturated hydraulic conductivity $K(\theta)$ in Eq. (2) is a function of soil water content θ. The relationship between $K(\theta)$ and θ is characterized by empirical formulas for the purpose of simplifying calculation and eliminating the needs of soil hydraulic parameters. These empirical formulas are referred to as drainage functions, and the commonly used ones

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can be found in Mao et al. (2018). The diffusion equation (Eq. 4) can be discretized using an implicit finite difference method, and then solved with the chasing method. An empirical formula with four parameters (saturated hydraulic conductivity K_s, saturated water content θ_s, field capacity θ_f, and residual water content θ_r) is used in Mao et al. (2018) to describe the hydraulic diffusivity $D(\theta)$. These parameters have physical meanings, and are easy to be obtained for large-scale modeling. A correction term is introduced to describe the spatial variability of soils, which makes the model applicable to heterogeneous situations. Both the upward and downward soil water movement can be simulated by UBMOD, and mass balance is well maintained by the model. The model can effectively and efficiently capture the features of soil water movement with coarse discretization in space and time.

2.2 The Brief Introduction of MODFLOW and Two Peripheral Tools

MODFLOW is a computer program that numerically solves the 3-D groundwater flow equation for a porous medium using a block-centered finite-difference method (Harbaugh, 2005). The governing equation solved by MODFLOW is

$$\frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial H}{\partial x_j}\right)+W=S_s\frac{\partial H}{\partial t}, \tag{5}$$

where $i = 1 - 3$ indicates the x, y, and z directions, respectively; K_{ij} is the saturated hydraulic conductivity [LT^{-1}]; H is the hydraulic head [L]; W is a volumetric flux per unit volume representing sources and/or sinks of water [L^3T^{-1}]; S_s is the specific storage of the porous material [L^{-1}]; and t is the time [T].

FloPy and ArcPy are the two peripheral tools used in our model development.

FloPy (Bakker et al., 2016) is a Python package for creating, running, and post-processing MODFLOW-based models. Unlike the commonly graphical user interfaces (GUIs) method, FloPy facilitates user to write a Python script to construct and post-process MODFLOW models, and it has been shown as a convenient and powerful tool by Bakker et al. (2016). Geographic information system (GIS) is a helpful tool for groundwater modeling by providing geospatial database and results presentation (Xu et al., 2011; Lachaal et al., 2012). ArcPy is an application program interface (API) of ArcGIS for Python (Toms, 2015), which provides a useful and productive way to perform geographic data analysis, data conversion, data management, and map automation with Python.

2.3 The Procedures of the New Model and the Modeling Framework

The schematic procedures of the modeling framework are shown in Fig. 1(a), which are composed of three major parts, including the pre-processing, the coupled model, and the post-processing. Two Python scripts are developed to facilitate the pre-processing and post-processing respectively. The coupling scheme is also realized using the Python script, while UBMOD and MODFLOW are used as the executable programs. The structure of the framework makes it flexible and expansible, as each component can be easily updated or replaced.

The preparation of geographic input information of the model shown in Fig. 1(b) is the major component of pre-processing. The geographic information includes the domain area, boundary conditions, sub-areas, digital elevation model (DEM), hydraulic conductivity and porosity. The shapefile of the domain area (usually irregular in shape) is first discretized by regular boundary with both active and inactive cells. The discretized domain can be joined with the shapefile of boundary condition to generate the "ibound" array of MODFLOW as shown in Fig. 1(b), which is used to specify which cells are active, inactive, or fixed head in MODFLOW. The shapefile of sub-areas is joined with the domain file, represented in subareas array with different number specified as different sub-areas. The raster files of DEM, hydraulic conductivity and porosity are further joined, and the values of these variables are listed in the arrays shown in Fig.1 (b). These procedures are implemented automatically by the help of the pre-processing tool developed by using ArcPy, FloPy and other Python packages. All these arrays including the geographic information are used by the coupled model for numerical simulation. The unsaturated-saturated flow model coupling scheme will be described in next section. The results presentations are accomplished in post-processing process by post-processing tool, which contains a series of utilities developed based on Python packages (NumPy, Pandas, Matplotlib, FloPy and other packages)

2.4 Coupling Scheme of UBMOD and MODFLOW

Figure 1(c) demonstrates the sketch map of the specific unsaturated and saturated coupling scheme. The unsaturated-saturated domain is partitioned into a number of sub-areas in the horizontal direction mainly according to the spatially distributed inputs (each sub-area is considered to be homogeneous in horizontal). Soil water flow of each sub-area is simulated by using one 1-D soil column. The whole saturated zone is

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discretized into a grid with cells, as shown in Fig. 1(c). All cells in the same sub-area receive the same recharge from soil zone calculated by the representative 1-D soil column of the sub-area. While it is feasible to use one soil column for each cell, this is impractical for most large-scale situations due to unavailable soil data and heavy computation cost. In the vertical direction, both the saturated domain and the soil columns are discretized into different layers based on available data and information, and the layer discretization remain unchanged during the simulation. Note that the saturated zone and the unsaturated zone are independent, but some layers may transform between the saturated zone and the unsaturated zone, which are referred as the overlap region. It should ensure that both the discretization and input information for saturated calculation and unsaturated calculation of the overlap region are assigned. As shown in the Fig. 1(c), there are m rows and n columns cells of the saturated zone, and l sub-areas, j layers for one soil column. The vertical layers for different soil columns can be different.

Since the output variable of UBMOD is the soil water content and the output of MODFLOW is hydraulic head, this study uses the vertical net recharge and the unsaturated zone depth to couple the unsaturated zone and saturated zone. The vertical net recharge is represented by matrix $\mathbf{R}$ with $m \times n$ elements, and the unsaturated zone depth by vector $\mathbf{Du}$ with l elements, as illustrated in Fig. 1(c). Scalar R is used in this study to denote the specific net recharge of a soil column to the corresponding saturated sub-area, scalar du is used to denote the depth of a soil column. A new method is developed to capture the net recharge between unsaturated zone and saturated zone. Figure 2(a) shows the spatial coupling scheme of a soil column connected with groundwater system. The water table locates in layer j. The net recharge R from unsaturated zone is calculated via

$$R = q_{\mathrm{I}} + q_{\mathrm{A}} - q_{\mathrm{S}} - q_{\mathrm{D}}, \tag{6}$$

where q_{I} is the flux across the water table caused by allocation of the infiltration water per unit area [L]; q_{A} is the flux across the water table caused by the advective movement per unit area [L]; q_{S} is the flux across the groundwater table caused by source/sink terms per unit area [L] and q_{D} is the flux across the water table caused by the water diffusion per unit area [L]. All the q terms are calculated by UBMOD.

Specifically, the infiltration water is allocated first according to the Eq. (1) if there is precipitation or irrigation. If there is a residual infiltration across the water table in the j layer of the unsaturated zone, the amount of residual infiltration is denoted as q_{I}. Then the advective flow q_{A} across the water table driven by gravitational potential is calculated by using Eq. (2). The directions of these two terms are downward. The q_{S} term is upward and resulted from groundwater by evapotranspiration. A virtual layer is needed when calculating the diffusive movement driven by matrix potential across the water table based on Eq. (4). As shown in Fig.2 (a), the virtual layer will be added under water table, numbered as layer j+1. The thickness, M_{j+1} [L], of the layer is set as,

$$M_{j+1} = z_{j+1} - d_u, \tag{7}$$

where z_{j+1} is the bottom depth of layer j+1 [L]. The amount of the upward flux between the virtual layer and layer j is denoted as q_D. Then, the net recharge matrix $\mathbf{R}$ for the whole area is obtained and used for the Recharge (RCH) package of MODFLOW.

The serial coupling scheme is shown in Fig. 2(b). There are three levels of time discretization in the coupling model (shown in Fig.2(b)) as follows: the stress periods ΔT used in MODFLOW, the time step Δt_s in each stress period during the saturated calculation, the time steps Δt_u during the unsaturated calculation. The unsaturated zone and saturated zone exchange information at the end of each stress period. Figure 2(c) describes the calculation procedures of the model and the iterative coupling scheme at time t. The model first reads the inputs of spatial data, prepares the model data and parameters, and updates the data at the beginning of the time or iteration loop. Then the model runs the UBMOD model with the unsaturated time step Δt_u to obtain the vertical recharge. The total recharge during the time level of stress period ΔT can be obtained by summarizing the recharge at each time step. The net recharge at time t and at the p-th iteration is represented as $\mathbf{R}_p$, which used by the MODFLOW RCH package. Subsequently, the model runs the MODFLOW model to obtain the saturated hydraulic head, $\mathbf{H}_t^p$ ($m\times n$ dimension), at time t and at the p-th iteration. The convergence of the iteration is determined by using the difference of hydraulic head between the present $\mathbf{H}_t^p$ and the previous iteration $\mathbf{H}_t^{p-1}$. The convergence criterion is

$$if \ \max\left(\left|\mathbf{H}_t^p - \mathbf{H}_t^{p-1}\right|\right) < \varepsilon_H , \tag{8}$$

where ε_H is a user-specified tolerance [L]. If the criterion is met, the iteration stops, and $\mathbf{H}_t^p$ is the convergent results at time t, and the model proceeds to the next time step.

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Otherwise, the iteration continuous to p+1. The unsaturated depth $\mathbf{Du}_t^{p+1}$ is updated at each iteration. Vector $\mathbf{Hs}_t^p$ (l dimension) is used to represent the average saturated hydraulic head over the same sub-area according to $\mathbf{H}_t^p$. Then the new unsaturated depth $\mathbf{Du}_t^{p+1}$ is calculated as follows

$$\mathbf{Du}_t^{p+1} = \mathbf{D} - \mathbf{Hs}_t^p , \tag{9}$$

where $\mathbf{D}$ (l dimension) is the average depth from the soil surface to the bottom in the same sub-area [L]. $\mathbf{Du}_t^{p+1}$ is set as the input to UBMOD, and the model proceeds to the next iteration until the convergence creation of Eq. (8) is met.

3 Model Evaluation

In this section, two test cases were designed to evaluate the model accuracy and the performance of the numerical coupling scheme under complicated soil and boundary conditions. The simulation results were compared with numerical results obtained using HYDRUS-1D (Šimůnek et al., 2008) and SWMS2D (Šimůnek et al., 1994), and with published experimental data. For these cases, the mean absolute relative error (*ARE*) and the root mean squared error (*RMSE*) were used to quantitatively evaluate the misfit between the simulated results of the developed model and reference values. *ARE* and *RMSE* are calculated as,

$$ARE = \frac{1}{x}\sum_{i=1}^{x}\frac{|y_i - Y_i|}{Y_i} \times 100\% , \tag{10}$$

$$RMSE = \sqrt{\frac{1}{x}\sum_{i=1}^{x}(Y_i - y_i)^2} , \tag{11}$$

where the subscript i represents the serial number of the results; x represents the total

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number of the results; y_i is the simulated result of the coupled model and Y_i is the reference result.

3.1 Two Test Cases

3.1.1 Case 1: 1D upward flux with atmospheric condition

This case was to test the performance of the coupling scheme explained in Sect. 2.4. It considered 1-D water flow in a field profile of the Hupselse Beek watershed in the Netherlands, which was used as a demo in HYDRUS-1D technical manual (Šimůnek, 2008). The soil profile consists of a 0.4m-thick upper layer and a 1.9m-thick bottom layer. The depth of the root zone is 0.3 m. The hydraulic parameters of the two soil layers are presented in Table 1. The surface boundary condition involves actual precipitation and potential transpiration rate as shown in Fig. 3. The groundwater level was initially set at 0.55 m below the soil surface. Only one vertical soil column and one MODFLOW cell were used in the coupled model. The parameters used in the coupled model are also listed in Table 1. The stress period ΔT was set as 5 d, and the MODFLOW time step Δt_s and the UBMOD time step Δt_u were both set to be 1 d. The results from HYDRUS-1D were used as the reference of this test case. The mean time step used in the HYDRUS-1D was 0.13 d. The spatial discretization of UBMOD was 0.1 m, and that of HYDRUS-1D varied between 0.01 m and 0.1 m.

3.1.2 Case 2: Two-dimensional (2D) water table recharge experiment

This test case was used for model validation in a 2-D unsaturated-saturated flow system. The numerical simulation of our model was compared with the data of a 2-D water table recharge experiment conducted by Vaulin et al. (1979). The experimental data have been used to test the variably saturated flow models (Clement et al., 1994) and coupled unsaturated-saturated flow models (Thoms et al., 2006; Twarakavi et al., 2008; Shen and Phanikumar, 2010; Xu et al., 2012). The 2-D domain is a rectangular sandy soil slab of 6.0 × 2.0 × 0.05 m. The initial pressure head is 0.65 m at the domain bottom. At the soil surface, a constant flux of q = 3.55 m/d is applied at the central 1.0 m, and the rest soil surface is the no flux boundary. Because of the symmetry of the flow system, only one half of domain (right side) with the size of 3.0 m × 2.0 m × 0.05 was simulated. The setup of the simulation is shown in the Fig. 4(a). No-flow boundaries were defined on the bottom and the left side, and specified hydraulic head boundary of 0.65 m was set on the right side. The values of soil hydraulic parameters are listed in Table 1. The simulation period is 8 h. In our coupled model, there were 30 uniform rectangular cells used by MODFLOW, and there were 10 sub-areas defined to represent the unsaturated zone, which were numbered from left to right. The first and last sub-areas covered 0.2 m and 0.4 m in the x direction respectively, and each the rest sub-area covered 0.3 m in the x direction. The first and the second sub-areas were used to define the recharge boundary, while the others sub-areas were used to define the no-recharge boundary. The stress period ΔT was set as 1 h, and the MODFLOW time step Δt_s and UBMOD time steps Δt_u were set as 0.167 h. The spatial discretization of UBMOD was uniformly 0.1 m. The experiment was also simulated by using SWMS2D, which considered the lateral flow. The mean time step of SWMS2D was set to be 0.0225 h, and 20, 200 finite elements were used.

3.2 Results and Discussions of Model Performance

3.2.1 Computational accuracy of the coupling scheme

Figure 5 shows the comparison of the results simulated by HYDRUS-1D and the coupled model of case 1. Figure 5(a) demonstrated that the water table depth calculated by the coupled model has a similar pattern to that of HYDRUS-1D. The *ARE* and *RMSE* values were 14.2% and 0.135 m, respectively. The soil water contents at the depth of 1.15m over time from the two models are compared in Fig. 5(b). The *ARE* and *RMSE* at z = 1.15 m were 1.9% and 0.008 cm^3/cm^3. The simulated soil water content profiles at different times are shown in Fig. 5(c). The *ARE* and *RMSE* values of different times were 2.2%, 5.6%, 6.0% and 0.017 cm^3/cm^3, 0.017 cm^3/cm^3, 0.018 cm^3/cm^3, respectively. These results indicate that the coupled model can capture the flow information under an upward flux and the heterogeneous condition.

Figure 4(b) shows the comparison of simulated water tables at 4 different times using the coupled model and SWMS2D and the observation data in case 2. The *ARE* and *RMSE* values are listed in Table 2. The coupled model matched the observation data well at the simulation times of 3 h, 4 h and 8 h, with the *ARE* values smaller than 3% and the *RMSE* values smaller than 0.03 m. The observed and simulated soil water content profiles for the initial and ending times are presented in Fig. 6. The *ARE* and *RMSE* values are also listed in Table 2. The SWMS2D model predicted accurately at all the locations. The simulations by the coupled model agreed well with the observations at the locations of $x = 0.2$ m, $x = 1.4$ m and $x = 2$ m (Figs. 6(a), (d) and (e)) where the lateral water flow was negligible. These results demonstrated the accuracy of the coupled model and the reliability of the coupling scheme shown in Sect. 2.4.

3.2.2 Limitations of the coupled model

Although the coupled model had a sufficient computational accuracy as shown above, there were limitations because of the quasi-3D assumptions. The coupled model overestimates the water table at the time of 2 h in case 2 as shown in Fig. 4(b). This was caused by a significant lateral flow in the unsaturated zone during the early period due to the relatively low initial soil water content condition. Therefore, a portion of the infiltration water in the first and second sub-areas should move in the lateral direction, instead of moving downward to the saturated zone as in the Quasi-3D model. The coupled model thus overestimated the recharge flux, and resulted in a higher water table at the early period. The *ARE* of groundwater table prediction of coupled model was 11.6% and *RMSE* 0.088m at the simulation time 2 h, which was larger than that of SWMS2D. Additionally, the simulated soil water content by the coupled model had poor performance at the locations of $x = 0.6$ m and $x = 0.8$ m (Fig. 6(b) and (c)). The *ARE* values of the coupled model were 80.5% and 52.1% at $x = 0.6$ m and $x = 0.8$ m, which were 11.4% and 21% in the SWMS2D. These two sub-areas were close to the recharge zone and affected by the lateral flow, which was ignored in the coupled model. Therefore, the coupled model overestimates the recharge and underestimates the soil water content when the lateral flow cannot be ignored. Its application should be limited

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to cases in which the soil flow mainly occurs in the vertical direction.

3.2.3 Water mass balance and computational cost

The mass balance error of the coupled model was small and the maximum value was 0.0063% in case 1 and 0.0037% in case 2, while it was 1.6% for the HYDRUS-1D model and 0.133% from the SWMS2D model. The cases were run on a 6 GB RAM, double 2.93 GHz intel Core (TM) 2 Duo CPU-based personal computer. For case 1, the simulation time of the coupled model and the HYDRUS-1D model were 81 s and 1.4 s, respectively. The iteration and information exchange were responsible for the high computational cost. For case 2, the simulation time of the coupled model and the SWMS2D model were 46 s and 95 s, respectively. The coupled model had a better efficiency comparing with the complete 2D model due to its simpler numerical solutions and coarse discretization in space and time. Therefore, the coupled model provided satisfactory mass balance and good computational efficiency.

4 Real-World Application

4.1 Study Site and Input Data

The coupled model was used to calculate the regional-scale groundwater recharge in a real-world case, where the shallow groundwater has significant impact on the soil water movement in the study site. Therefore, the widely adopted methods (e.g., such as INFIL 3.0 developed by Fill (2008)) estimating groundwater recharge without concerning the groundwater movement may be inadequate for the recharge estimation. Figure 7(a) shows the location of the study site, the Yonglian irrigation area (107°37′19″

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- 108°51′04″ E, 40°45′57″ - 41°17′58″ N) in Inner Mongalia, China. The irrigation area is 12 km long from north to south, and 3 km wide from east to west. The whole domain size is 29.75 km^2. The ground surface elevation decreases from 1028.9 m to 1025.4 m from the southwest to the northeast. A two-year tracer experiment from 2014 to 2016 was conducted to obtain the groundwater recharge (Yang, 2018), and the experimental locations are shown in Fig. 7(a). This irrigation area has well-defined hydrogeological borders by the channel network. Since the Zaohuo Trunk Canal and No. 6 Drainage Ditch are filled with water over the simulation time, the first-kind boundary condition was applied to the two segments. The non-flow boundary condition was used for the other segments of the area. The irrigation water of this area is diverted from the Renmin Canal. This irrigation area was divided into three sub-areas according to the land uses at the site, which were farm land, villages and bared soil, as shown in Fig. 7(b). The crop types in the farmland were not considered for determining the sub-areas. The surface digital elevation model (DEM) is shown in Fig. 7(c).

The measured soil water content and groundwater table in the crop growing season from May to October of 2004 were used to calibrate the hydraulic parameters, and the tracer experiment from 2014 to 2016 was used for the groundwater recharge evaluation. A uniform daily rainfall rate was applied to the whole domain. The irrigation water was only applied to the farm land. The potential evapotranspiration ET_0 in 2004 was calculated by the measured evaporation data from the 20 cm pan, multiplying by the conversion coefficient of 0.55 recommended by Hao (2016). The ET_0 during 2014 to

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2016 was calculated by using the Penman-Monteith equation. The precipitation, irrigation and ET_0 are shown in Fig. 8. The crop growing season is from May to October, and the rest months are no-crop growing season. Based on the hydrogeological characteristics of the study area provided by the Geological Department of Inner Mongolia, the top aquifer within the depth of 7 m is loamy sand and loam with small hydraulic conductivity; an underlying sand aquifer with the thickness of 46 m has high permeability, and the sand aquifer is lying on an impervious 1m-thick clay layer. The clay layer was used as the bottom of the simulation domain, and seven different geological layers were used in the MODFLOW model. The first layer was set to be the top aquifer, and the second aquifer were divided into 6 layers for numerical simulation. Ten groundwater monitoring wells were set in this district, and the groundwater tables were observed every 6 days. Well 1, well 2, well 3, well 5 and well 6 are located in the farm land area, well 4 and well 8 in a village, and well 7, well 9 and well 10 in a bared soil area. Additionally, there are 5 soil water content monitoring points in the farm land and 2 points in the bared soil area, as shown in Fig.7(a). Soil water contents within 1 m depth were observed 1-3 times every month from May to October in 2004.

Five GIS files are prepared as the shapefile files of the study domain, the land use types, the boundary conditions, and raster files of the surface DEM and initial hydraulic head. There were 150 rows and 50 columns used in the MODFLOW model. The spatial discretization of UBMOD was set to be 0.1 m. The stress period ΔT was set as 5 d, and the MODFLOW time step Δt_s and UBMOD time step Δt_u were set as 1 d.

4.2 Model Calibration Results

There were two soil types in the first layer as loamy sand and loam. The unsaturated hydraulic parameters of the two soils are listed in Table 3. The hydraulic conductivity of the top aquifer in MODFLOW was set as the same as the unsaturated layer, the hydraulic conductivity of the bottom sand aquifer was set as 3.5 m/d during the calibration, and the specific yields of the top and bottom were set as 0.08 and 0.1, respectively. Figure 9 shows the comparison of the simulated and observed water table depth for the four areas, i.e., the whole area, farm land, village, and bared soil. The measured water table depths were averaged according to the land use types. The *ARE* values of four areas are 17.1%, 20.0%, 21.2%, 23.0%, respectively, and the *RMSE* values of the four areas are 0.306 m, 0.261 m, 0.421 m, 0.428 m, respectively. Figure 10 further shows the spatial distribution of the simulated water table depth at different output times. The increase trend is obviously found from Fig. 10(a) to Fig. 10(c) in the farm land, during which the groundwater was consumed by crop transpiration and soil evaporation, while slight changes are found in the non-farm land. When the intensive autumn irrigation happened after the 160th day, the water table depth in the farm land decreased rapidly, as shown in Fig. 10(d). These results indicate that our model can reasonably simulate the saturated water table depth in space and time.

Figure 11 shows the comparison between the simulated and average observed soil water content profiles of the farm land and bared soil at different times. The *ARE* values of the farm land at the times of 40d, 85d, 125d, and 166d were 26.2%, 24.4%, 27.5%, 29.1%, respectively, and the *RMSE* values of the four times are 0.009 cm^3/cm^3, 0.073 cm^3/cm^3, 0.083 cm^3/cm^3, 0.088 cm^3/cm^3, respectively. The corresponding values for the bared soil were 15.5%, 18.1%, 12.8%, 14.0% and 0.055 cm^3/cm^3, 0.055 cm^3/cm^3, 0.041 cm^3/cm^3, 0.032 cm^3/cm^3, respectively. The observations had higher soil water content in the root zone than those from the simulations in the farm land. The sampling points located at the border of fields, which leads to an overestimation of the soil water content in the root zone due to less crop root uptake. The simulated soil water content profiles in the bared soil agreed well with the observations.

4.3 Regional Groundwater Recharge

In the tracer experiment, bromide (Br) was used as the tracer for calculating groundwater recharge. The tracer was injected at 1 m depth at two points shown in Fig. 7(a) in October, 2014. Based on two sampling in October of 2015 and 2016, the downward recharge is estimated according to the movement of the tracer peak. As shown in Table 4, the annual average recharge *R* was 33.8 mm/year, and the recharge coefficient was 0.055 during the period of 2014 - 2016.

The calibrated coupled model was used to estimate the groundwater recharge from October 1, 2014 to September 30, 2016. Figure 12 shows the time series of simulated recharge rate in the farm land, and Table 4 lists the simulation results. The simulation results indicate that groundwater is recharged in the no-crop growing season and consumed in the crop growing season. The two peak values of groundwater recharge in

Fig. 12 are due to the autumn irrigation after harvest for washing salt out. The no-crop growing season provided 66.3 mm/year groundwater recharge over a year and the average recharge coefficient was 0.249, which indicates that the autumn irrigation in the no-crop growing season provided the primary groundwater recharge in the year. In the crop growth season, the recharge was negative, which meant that groundwater was consumed by crop transpiration and soil evaporation. As calculated by the coupled model, the annual groundwater recharge was 28 mm/year during the period from October 1, 2014 to September 30, 2016 in the farm land, which was similar to the result of the tracer experiment. The results confirmed the coupled model for groundwater recharge evaluation, which was helpful for scheduling the irrigation amount in the crop growing season under the water saving policies.

5 Conclusions

This study developed a new Quasi-3D coupled model for the purpose of practical modeling of unsaturated-saturated flow at the regional scale. The 1-D water balance model UBMOD describing the unsaturated soil water flow was integrated with MODFLOW iteratively. A developed framework implemented the modeling procedures, and provided the pre- and post-processing tools. The model was evaluated by using both synthetic numerical examples and real-world experimental data. The major conclusions drawn from this research are as follows,

(1) The new iteration coupling scheme iteratively integrating a hydrodynamic model

with a water balance model is reliable. The vertical net recharge and the depth of the unsaturated zone are effective to be used as the exchange information to couple the unsaturated zone and saturated zone.

(2) The satisfactory results in the two testing examples demonstrate the effectiveness of the new Quasi-3D model with an acceptable calculative efficiency and well maintained mass balance.

(3) The model gives a satisfactory performance for calculating the groundwater recharge measured from the tracer experiment. The calculated annual groundwater recharge is 28 mm/year and the recharge coefficient is 0.046 in the study area.

(4) The proposed framework makes the model easy to be expanded, and it gives a complete solution from geographic information preparation to results displaying simply and conveniently, even for a complex practical problem.

(5) The coupled model should not be used for problems with substantial lateral flow in the unsaturated zone because of the quasi-3D assumptions used in the model.

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Table 1. The hydraulic parameters of case 1 and case 2.

	Depth (m)	The parameters used by HYDRUS-1D/SWMS2D and the coupled model			The parameters used only by HYDRUS-1D/SWMS2D		The parameters used only by the coupled model	
		θ_r (-)	θ_s (-)	K_s (m/d)	n	α (1/m)	θ_f (-)	μ
Case 1	0-0.4	0.001	0.399	0.2975	1.3757	1.74	0.26	-
	0.4-2.3	0.001	0.339	0.4534	1.6024	1.39	0.22	0.1
Case 2	0-2.0	0.001	0.3	8.4	4.1	3.3	0.15	0.15

θ_r is the residual water content (L^3L^{-3}); θ_s is the saturated water content (L^3L^{-3}); K_s is the saturated hydraulic conductivity (LT^{-1}); α (L^{-1}) and n (-) are parameters depending on the pore size distribution; θ_f is the field capacity (L^3L^{-3}) and μ is the specific yield (-).

Table 2. The *ARE* and *RMSE* values of SWMS2D and coupled model of case 2.

Water table		t = 2 h	t = 3 h	t = 4 h	t = 8 h	
ARE (%)	SWMS2D	0.9%	1.5%	1.6%	1.8%	
	Coupled model	11.6%	2.4%	2.9%	1.6%	
RMSE (m)	SWMS2D	0.010	0.014	0.016	0.022	
	Coupled model	0.088	0.025	0.029	0.021	
Soil water content profile		x=0.2 m	x=0.6 m	x=0.8 m	x=1.4 m	x=2 m
ARE (%)	SWMS2D	5.6%	11.4%	21.0%	17.6%	6.7%
	Coupled model	12.3%	80.5%	52.1%	27.6%	4.1%
RMSE (cm^3/cm^3)	SWMS2D	0.018	0.031	0.044	0.022	0.017
	Coupled model	0.040	0.173	0.109	0.039	0.010

Table 3. The unsaturated hydraulic parameters.

Soil type	Location	θ_r (-)	θ_s (-)	K_s (m/d)	θ_f (-)
Loamy sand	Village, bared soils	0.065	0.41	1.061	0.18
Loam	Farm land	0.078	0.43	0.2496	0.25

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760 Table 4. The recharge sources and results of the tracer experiment.

	Tracer experiment	Coupled model		
		Crop growing season	No-crop growing season	Annual
P (mm/year)	133.55	100	33.55	133.55
I (mm/year)	477.52	244.27	233.25	477.52
R (mm/year)	33.8	66.3	-38.3	28
R_c (-)	0.055	0.249	-	0.046

761 Note: P is the annual precipitation; I is the irrigation water; R is the annual recharge and R_c is the
762 recharge coefficient, $R_c = R/(P+I)$.
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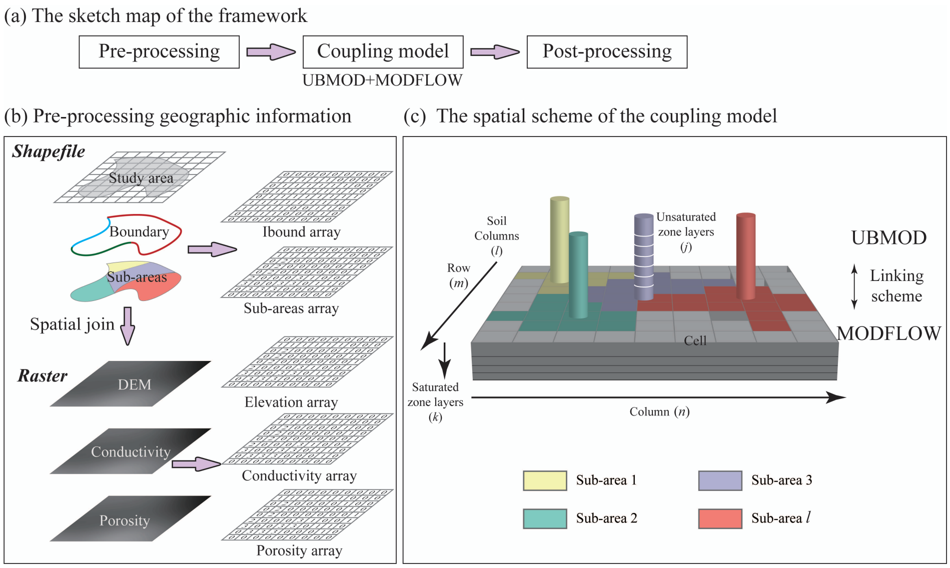

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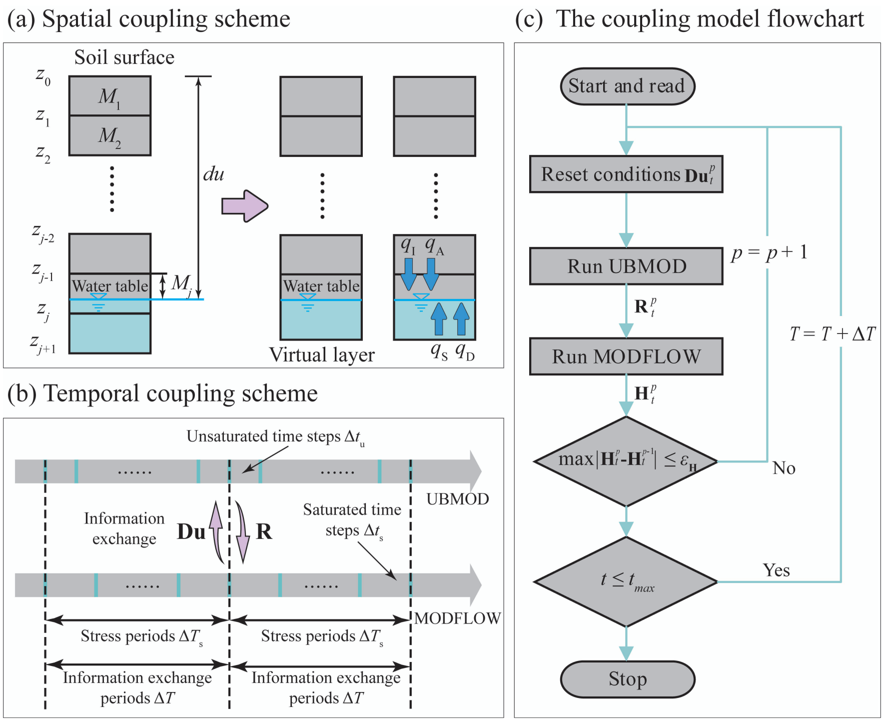

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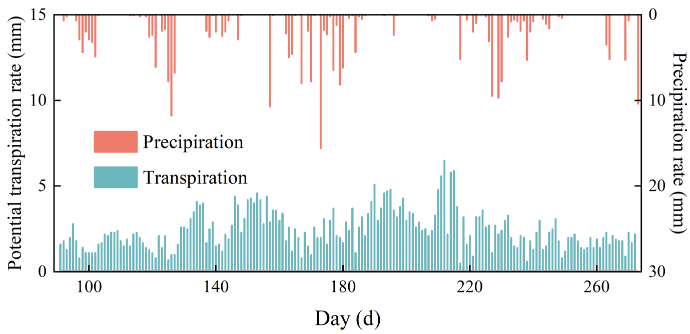

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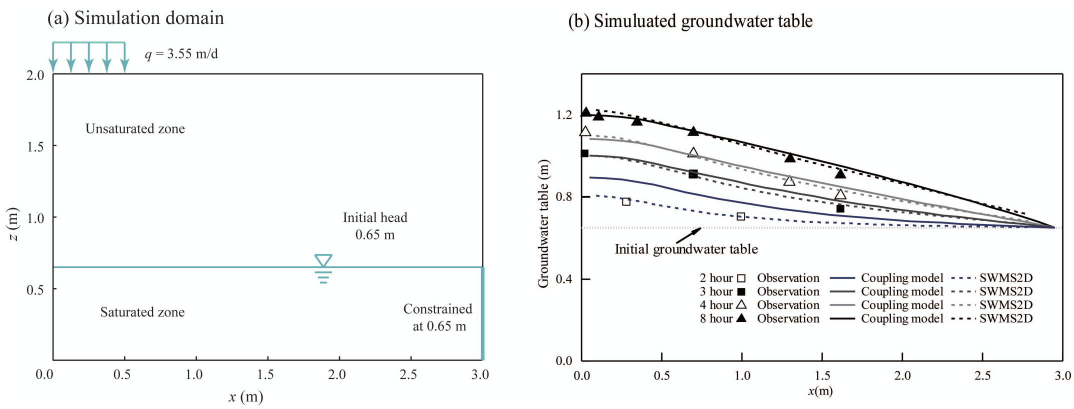

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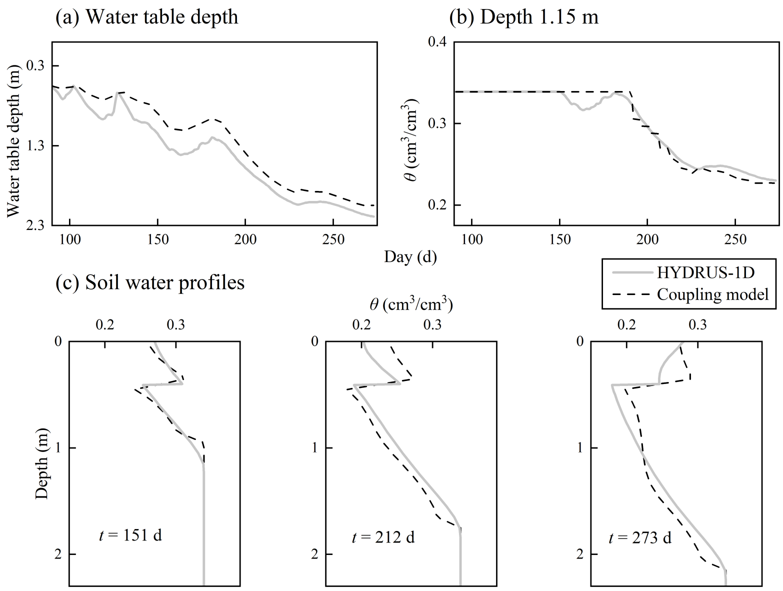

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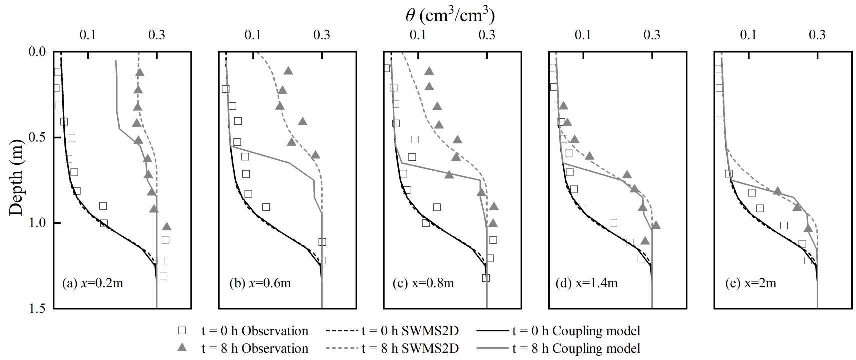

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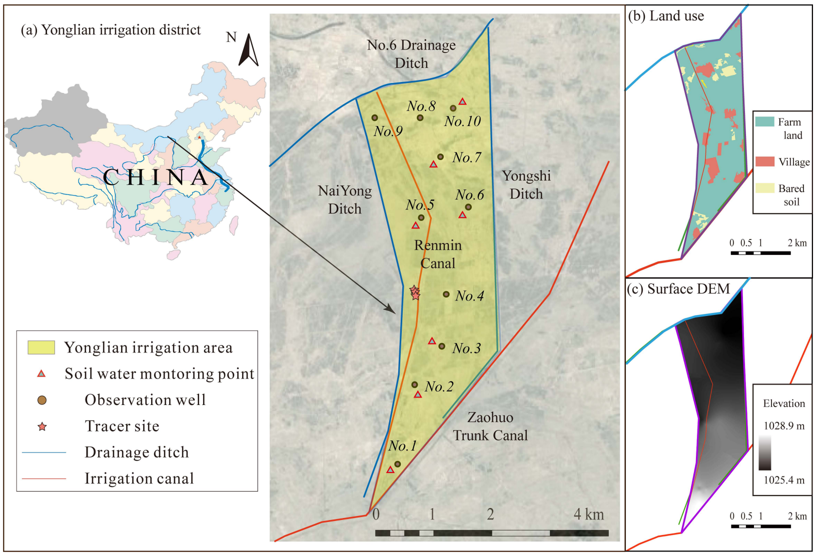

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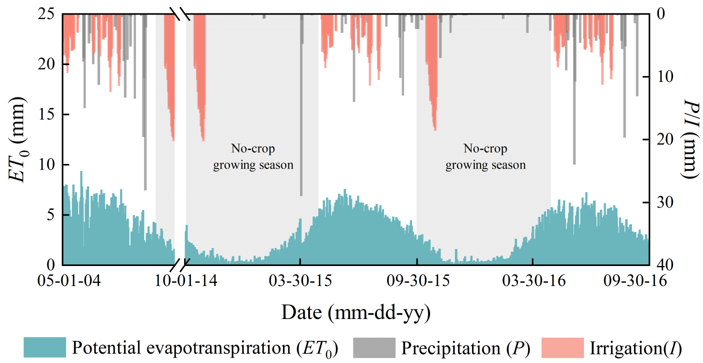

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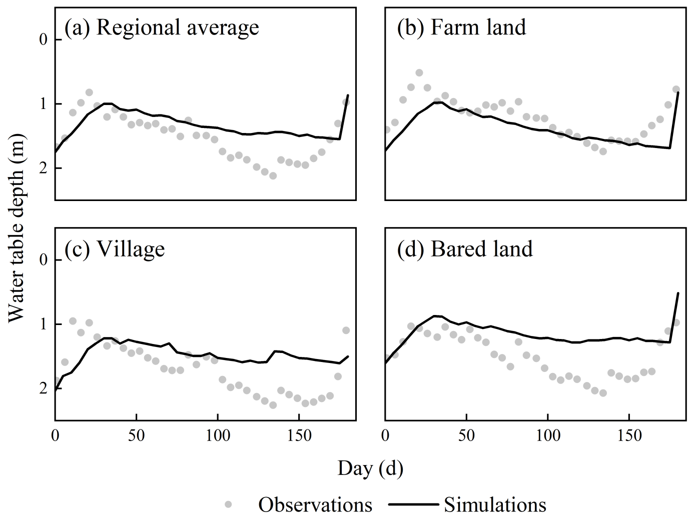

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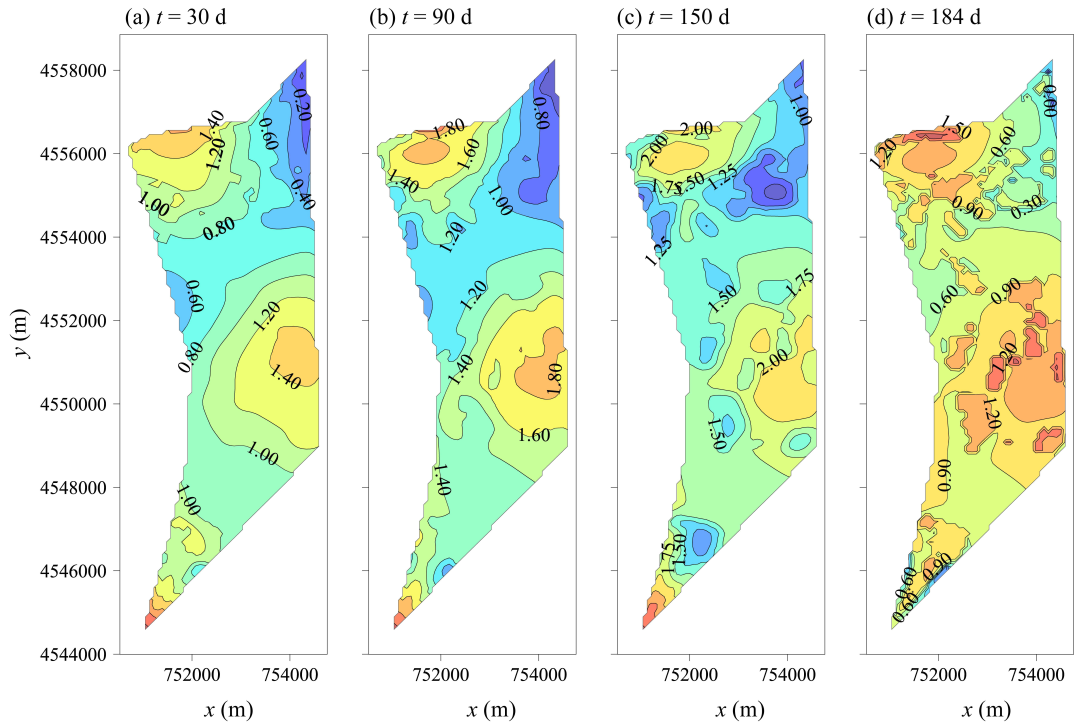

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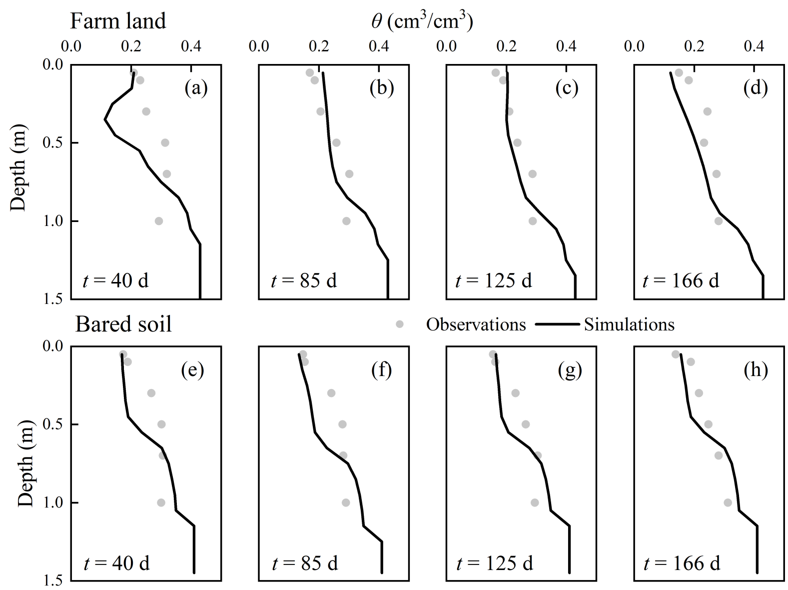

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816 Fig. 11. Comparison between simulated and observed regional average soil water content profile.

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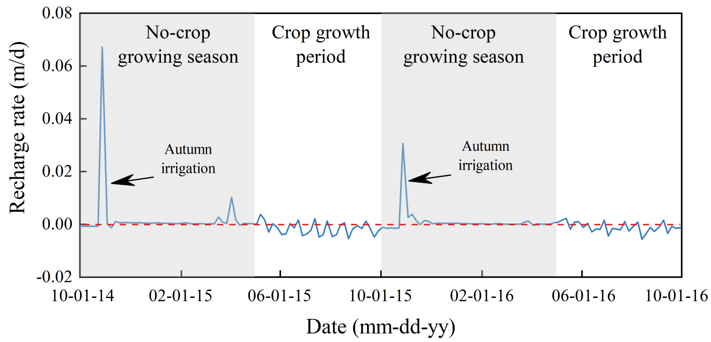

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