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Integration of SWAP and MODFLOW-2000 for modeling groundwater dynamics in shallow water table areas

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SUMMARY

Reasonable estimates of groundwater recharge and discharge through evapotranspiration is critical for sustainable water resources management in shallow water table areas. The hydrologic processes are highly interactive between the vadose zone and groundwater under shallow water table conditions. In traditional groundwater flow models, the recharge and evapotranspiration fluxes are often oversimplified as a simple sink/source term. However, the recharge and evapotranspiration are observed to vary with topography, soil type, land use, and water management practices. Additionally, they are known to vary temporally and spatially and are difficult to estimate, especially in arid and semi-arid regions. Thus, it is important to devise an appropriate method to estimate the recharge and evapotranspiration fluxes in groundwater modeling. In this study, a Soil–Water–Atmosphere–Plant (SWAP) package was integrated into a groundwater flow model (MODFLOW) in such a way that the SWAP package calculates vertical flux for MODFLOW, while MODFLOW provides averaged water table depth to determine the bottom boundary condition for SWAP zones. The SWAP zones in MODFLOW are derived from a combination of topology, soil type, land use, water management practices using geographic information systems (GIS). Then the MODFLOW with SWAP package was tested using a two-dimensional saturated–unsaturated water table recharge experiment. Results showed that the simulated water table elevations matched well with the observed ones except at the early period during which they were slightly higher than the observed ones, probably due to neglecting lateral diffusion in the unsaturated zone. Finally, we applied MODFLOW with SWAP package to simulate a regional groundwater flow problem in Hetao Irrigation District, upper Yellow River basin of North China. The simulation results validated the applicability of the developed MODFLOW with SWAP package for practical regional groundwater modeling.

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1. Introduction

Groundwater recharge and evapotranspiration (discharged by direct evaporation and crop root uptake through capillary rise) through the vadose zone are of great importance for sustainable groundwater use and control of salinity and water-logging in arid and semi-arid regions with shallow water tables (Lerner et al., 1990; Arnold et al., 1993). Salinity has affected at least 20% of the world's arable land and more than 40% of all irrigated land to various degrees (Rhoades and Loveday, 1990), especially in arid

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and semi-arid regions such as North China (Xu et al., 2010) and Southwest Australia (Petheram et al., 2003). Thus, reasonable estimates of groundwater recharge and evapotranspiration is significant for sustainable groundwater management. However, the groundwater recharge and evapotranspiration are influenced by a range of factors such as topography, soil type, land use, and water management practices (Petheram et al., 2003). The rates of recharge and evapotranspiration are known to be the most difficult and uncertain components to estimate in groundwater budget, and they often vary spatially and temporally, especially in arid and semi-arid regions (Hendrickx and Walker, 1997; Sophocleous, 2004). The traditional physical methods for recharge and evapotranspiration estimation such as direct measurement, water balances, Darcian approaches and empirical models often require large in situ measurement data, and are still limited to small scales (Sophocleous, 2004). The tracer techniques are successfully used to estimate the recharge in arid and semi-arid regions, but they also

only provide point or local scale information and do not directly quantify field scale recharge over a large area (Lerner et al., 1990). Recent developments in remote sensing techniques allow to map the groundwater recharge in a spatially distributed manner, as demonstrated by Brunner et al. (2004) or Tweed et al. (2007).

The groundwater recharge and evapotranspiration can also be estimated using physically-based numerical vadose zone model of which the principal advantages are that the models can allow reasonable forecast of the future recharge regimes under changing hydrological conditions such as changes in surface water management (Sophocleous, 2004; Allison et al., 1994). Most widely used groundwater flow models always oversimplify the estimates of groundwater recharge and evapotranspiration fluxes through vadose zone for regional groundwater flow simulation. They often treat the groundwater recharge and evapotranspiration loss as simple source terms with no interface, which underestimates the effects of vadose zone on groundwater flow system. For example, in some traditional groundwater flow models such as FEFLOW (Diersch, 1996) and PLASM (Prickett and Lonquist, 1971), these fluxes are often imposed by the modeler and estimated independently from the models when used for regional groundwater flow simulation. In MODFLOW-2000 (Harbaugh et al., 2000), the recharge rate is often directly specified by users as flux, and evapotranspiration is treated as a head-dependant flux boundary, using a linear or a piecewise linear relationship between water table depth and evapotranspiration rate. Sometimes, one also uses a continuous recharge–discharge function to represent groundwater discharge and recharge fluxes as a head-dependent continuous process (Doble et al., 2009). However, such an effort still may not appropriately estimate groundwater recharge and evapotranspiration for models due to the complex hydrological and environmental conditions in the vadose zone.

Although some variably saturated models such as MODFLOW-SURFACT (HydroGeoLogic Inc., 1996), VSF package (Thoms et al., 2006), HydroGeoSphere (Therrien et al., 2007) and HYDRUS (2D/3D) (Šimůnek et al., 2006) are able to describe the vadose zone water flow processes and estimate the recharge and discharge, they are all based on the use of three-dimensional Richards equations. Thus, it may impound heavily available computational resources to use these models due to the requirement of much finer temporal and spatial discretization (van Walsum and Groenendijk, 2008). In addition, some models do not reasonably consider the effects of vegetation growth and meteorological factors on groundwater recharge and evapotranspiration (such as VSF package), which have significant impacts on water flow in vadose zone. While others (e.g., HYDRUS-2D/3D) are not appropriate for regional groundwater flow modeling due to the limitation of dealing with the boundary conditions and source/sink terms. Considering the fact that water flow in vadose zone is usually assumed to be vertically one-dimensional (1-D) in field (Kroes and van Dam, 2003; Singh et al., 2006), therefore, it may be an alternative method to couple a 1-D vadose zone flow model into groundwater flow models through the exchange of information between these two models. This method has also been successfully applied in some previous studies. For example, Hollanders et al. (2005) applied a loose coupling, while van Walsum and Groenendijk (2008) used an online computational scheme for coupling SWAP and MODFLOW. The loose coupling is relatively easy to be realized, but it cannot characterize the timely interaction between groundwater flow and vadose zone flow. Some researchers (Stoppelenburg et al., 2005; van Dam et al., 2008) have employed an offline coupling which can iteratively solve the groundwater flow equation and Richards equation until their solutions converge. It may be very expensive when the iteration is involved on the equation level (Shen and Phanikumar, 2010). In addition, their coupling is based

on a specific assumption that a lower permeable layer underlies the unconfined aquifer, which is not always possible. Twarakavi et al. (2008) has fully coupled the simplified HYDRUS-1D and MODFLOW without considering the effects of vegetation and meteorological factors. Shen and Phanikumar (2010) have developed a coupling method which lowers the dimensions of 3-D Richards equation by separating it into 1-D equation for vadose zone flow and 2-D equation for groundwater flow.

Keeping the above in view, a 1-D vadose zone flow process, which comprehensively considers the effects of soil–plant–atmosphere continuum on groundwater dynamics, should be fully embedded into 3-D groundwater flow models. Therefore, the objectives of this study were to adapt the simplified Soil–Water–Atmosphere–Plant (SWAP) package from the original SWAP model (Kroes and van Dam, 2003) to simulate 1-D vertical flow in the vadose zone, and to couple the SWAP package with MODFLOW-2000 for appropriate estimation of groundwater recharge and evapotranspiration. They were coupled through the exchange of water table depth and net recharge, i.e., the difference between groundwater recharge and evapotranspiration. The coupled MODFLOW-2000 with the SWAP package was first tested using a well documented two-dimensional saturated–unsaturated water table recharge experiment (Vauclin et al., 1979). Then it was further validated by applying it to simulate the groundwater dynamics in an arid irrigation district on a regional scale. Consequently, this study was expected to extend the capabilities for MODFLOW to simulate groundwater dynamics.

2. Methodology

2.1. Description of MODFLOW-2000

MODFLOW is a computer program that numerically solves the three-dimensional groundwater flow equation for a porous medium using a finite-difference method (McDonald and Harbaugh, 1988) as follows:

$$\frac{\partial}{\partial x} \left(K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{yy} \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_{zz} \frac{\partial h}{\partial z} \right) - W = S_s \frac{\partial h}{\partial t}, \quad (1)$$

where K_{xx} , K_{yy} and K_{zz} are values of principal hydraulic conductivity along the x , y , and z coordinate axes (m d^{-1}), respectively; h is the potentiometric head (m); W is a volumetric flux per unit volume representing sources and/or sinks of water ($\text{m}^3 \text{d}^{-1}$); S_s is the specific storage of the porous material (d^{-1}); and t is time (d).

The MODFLOW-2000 is an updated version of MODFLOW-88 and MODFLOW-96. It consists of the global, groundwater flow, observation, sensitivity and parameter-estimation processes (Harbaugh et al., 2000). All these processes are further divided into independent subroutines or modules. These modules are grouped into packages which deal with specific aspects of the simulation. The modular structure of MODFLOW facilitates the development of other packages to freely handle the impacts of boundary conditions and sinks/sources. Visual MODFLOW which includes MODFLOW-2000, is a commonly used MODFLOW pre/post processor (Waterloo Hydrogeologic Inc., 2006), whose version 4.2 was employed in this study.

In MODFLOW, the Recharge (RCH) and Evapotranspiration (EVT) or Evapotranspiration Segments (ETS) packages (RCH-EVT or RCH-ETS) are widely used to characterize the vadose zone flow processes (Xu et al., 2011). The recharge rate is often directly specified by users as flux in the RCH package. While evapotranspiration is treated as a head-dependant flux boundary using a linear or several linear segments relationships between water table depth and evapotranspiration rate in MODFLOW-2000. The user-specified extinction depth and the maximum evapotranspiration

rate (at ground surface) are used in simulation. However, groundwater recharge and evapotranspiration through the vadose zone have both been observed to vary with water table depth, soil type, land use and water management practices. Therefore, the current MODFLOW-2000 still may not appropriately describe the effect of the vadose zone on groundwater flow system, due to the complex field conditions. The applicability of above mentioned methods is apparently questionable for arid and semiarid regions where soil capillary pressures play a dominant role in vadose zone flow (Lerner et al., 1990; Hendrickx and Walker, 1997).

2.2. SWAP package used for MODFLOW-2000

The groundwater recharge and evapotranspiration depend on topography, climate, soil, land use and water management practices which vary spatially and temporally on the regional scale. The SWAP model is a 1-D eco-hydrological model for simulating water flow, salt and heat transport in close interaction with crop growth in the vadose zone, which has been widely used for irrigation water management, salinity control and crop production prediction, etc. (Kroes and van Dam, 2003; Singh et al., 2006; Droogers et al., 2000). The SWAP package used here was simplified with removal of solute and heat transport modules, and then this package was adapted to simulate 1-D vertical transient saturated–unsaturated flow with considering the impacts of irrigation, rainfall, soil evaporation, runoff, drainage/sub-infiltration and crops root water uptake. The hysteresis, scaling of soil hydraulic properties, preferential flow and mobile/immobile flow were not considered in current version of SWAP package. When using the SWAP package, the simulation domain was divided into sub-regions (i.e., SWAP zones) analogous to the zones used in RCH, EVT or ETS packages of MODFLOW-2000 (Xu et al., 2011). The approach used for defining the land use systems (LUS) (FAO, 1976) was adopted to determine the SWAP zones. Some results also indicated that the topography has significant influences on the estimation of groundwater evapotranspiration (Li et al., 2008). In this study, each SWAP zone was denoted as a spatially homogeneous region, which was obtained through combination of topography, soil types, land use, irrigation, climatic conditions and water table depth conditions (Fig. 1). The SWAP zones in polygon format can be constructed by overlapping the vector maps using ArcGIS software, and subsequently transforming the maps into an ASCII format matrix for MODFLOW-2000 use as described by Xu et al. (2009).

The calculation of vadose zone water flow was applied to each SWAP zone when using the SWAP package. In each SWAP zone, the water movement is described by a vertically 1-D Richards

equation (see Eq. (2)) which is subsequently solved using an implicit finite-difference scheme.

$$C(h) \frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left[K(h) \left(\frac{\partial h}{\partial z} + 1 \right) \right] - S_a(z), \quad (2)$$

where C is the differential soil water capacity (cm^{-1}), h is the soil water pressure head (cm), t is time (d), z is the vertical coordinate (cm, positive upward), K is the hydraulic conductivity (cm d^{-1}) and S_a is the soil water extraction rate by plant roots ($\text{cm}^3 \text{cm}^{-3} \text{d}^{-1}$). The sink term $S_a(z)$ refers to water stress described by a reduction function proposed by Feddes et al. (1978).

The soil hydraulic properties can be described using van Genuchten (1980) and Mualem (1976) functions, respectively:

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{(1 + |\alpha h|^n)^{(n-1)/n}}, \quad (3)$$

$$K(\theta) = K_s S_e^\lambda \left[1 - \left(1 - S_e^{n/(n-1)} \right)^{(n-1)/n} \right]^2, \quad (4)$$

where θ_r is the residual water content ($\text{cm}^3 \text{cm}^{-3}$), θ_s is the saturated water content ($\text{cm}^3 \text{cm}^{-3}$), θ is the actual soil water content ($\text{cm}^3 \text{cm}^{-3}$), α (cm^{-1}) and n (dimensionless) are empirical shape factors, K_s is the saturated hydraulic conductivity (cm d^{-1}), $S_e = (\theta - \theta_r)/(\theta_s - \theta_r)$ is the relative saturation, and λ is a shape parameter (dimensionless). A common method, which is the implicit, backward, finite-difference scheme with explicit linearization as described by Haverkamp et al. (1977) and Belmans et al. (1983), is adopted to solve Richards equation. In addition, adaptations relative to treatments of differential water capacity and hydraulic conductivity functions are made to obtain the numerical scheme by Kroes and van Dam (2003). The soil profile is vertically discretized into compartments with various thickness i.e., a 1-D finite-difference grid. A finer discretization should be used at locations where sharp pressure head gradients are expected, and this can ensure the convergence of the numerical solution (Kroes and van Dam, 2003; Twarakavi et al., 2008). For example, smaller thickness of compartment are usually needed when close to the soil surface where rapid changes in water content and pressure head gradients often occur due to the effects of meteorological factors (Šimůnek et al., 2005).

The top boundary condition can be determined by the actual evaporation and transpiration rates and the irrigation and precipitation fluxes. For appropriate estimation of the actual evaporation and transpiration rates, the potential evapotranspiration (ET_p , mm d^{-1}) is estimated first using the Penman–Monteith equation (Allen et al., 1998):

$$ET_p = \frac{\frac{\Delta_v}{\lambda_w} (R_n - G) + \frac{p_1 \rho_{air} C_{air}}{\lambda_w} \frac{e_{sat} - e_a}{r_{air}}}{\Delta_v + \gamma_{air} \left(1 + \frac{r_{crop}}{r_{air}} \right)}, \quad (5)$$

where Δ_v is the slope of the vapor pressure curve ($\text{kPa } ^\circ\text{C}^{-1}$), λ_w is the latent heat of vaporization (J kg^{-1}), R_n is the net radiation flux at the canopy surface ($\text{J m}^{-2} \text{d}^{-1}$), G is the soil heat flux ($\text{J m}^{-2} \text{d}^{-1}$), p_1 accounts for time unit conversion ($=86,400 \text{ s d}^{-1}$), ρ_{air} is the air density (kg m^{-3}), C_{air} is the heat capacity of moist air ($\text{J kg}^{-1} \text{ } ^\circ\text{C}^{-1}$), e_{sat} is the saturation vapor pressure (kPa), e_a is the actual vapor pressure (kPa), γ_{air} is the psychrometric constant ($\text{kPa } ^\circ\text{C}^{-1}$), r_{crop} is the crop resistance (s m^{-1}) and r_{air} is the aerodynamic resistance (s m^{-1}). The ET_p can also be directly calculated by the product of the user-specified reference evapotranspiration (ET_{ref}) and the crop factors in absence of climatic or crop data. Potential evapotranspiration is then partitioned into potential soil evaporation and crop transpiration by using the leaf area index or soil cover fraction. Root water extraction at various depths in the root zone is calculated from the potential transpiration, root-length density and possible reduction from wet or dry conditions. In dry soil conditions, the

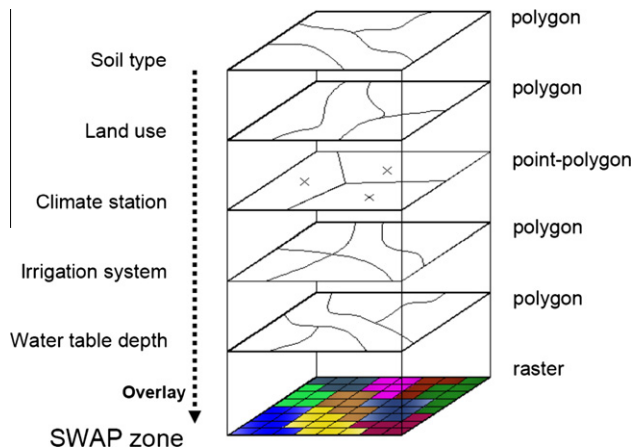


Fig. 1. Schematic description of SWAP zones in the SWAP package.

maximum evaporation rate, E_{max} (cm d⁻¹), is calculated according to Darcy's law (van Dam et al., 1997). As the actual soil evaporation may be overestimated using Darcy's law, two empirical exponential functions of Black et al. (1969) and Boesten and Stroosnijder (1986) are alternatively applied to calculate the actual evaporation, E_{aem} (cm d⁻¹). These two empirical functions are both used to estimate the cumulative actual evaporation during a dry cycle and then to obtain the daily actual evaporation. Finally, SWAP determines the actual evaporation rate by taking the minimum value of E_{max} and E_{aem} .

Surface runoff is simulated when the infiltration capacity of the soil is not sufficient to infiltrate all the water. The excess water on the soil surface builds up as a ponded reservoir until the pond water level exceeds a certain threshold ponding level (h_{pond}), which leads to the following surface runoff as:

$$q_{runoff} = \frac{1}{\gamma_{sill}} (h_{pond} - Z_{sill})^{\beta_{sill}}, \quad (6)$$

where q_{runoff} is the surface runoff (cm d⁻¹), h_{pond} is the ponding depth of surface water (cm), Z_{sill} is the height of the sill which is equal to the maximum ponding height specified by user (cm), γ_{sill} is the runoff/inundation resistance (d) and β_{sill} is an exponent (-).

The SWAP package provided options to prescribe the lower boundary conditions of soil profile as either the Dirichlet type (given pressure head), or Neumann type (given flux). When a shallow water depth condition existed, the bottom boundary pressure head value of soil profile can be determined according to averaged water table depth of the SWAP zone as follows:

$$h_{n,i} = GWL_i - z_{n,i} - h_{resis,i}, \quad (7)$$

where $h_{n,i}$ is the pressure head at the bottom of the soil profile (cm), GWL_i is the groundwater level (negative = below surface level, cm), $z_{n,i}$ is the position of bottom nodal point (negative, cm), $h_{resis,i}$ is the head difference between the groundwater level and hydraulic head of the bottom nodal point in the previous time step, the subscript i is the number of the SWAP zone and the subscript n represents the number of the bottom nodal point. If water table was deep and lower than the bottom of soil profile, the free drainage boundary condition at bottom of soil profile was provided for the SWAP zone.

The basic drainage module was used to describe the drainage/infiltration processes at the field scale in this study. The interaction between groundwater and up to five surface water systems, including drainage ditches and canals, can be simulated as follows:

$$q_{drain,i} = \frac{\phi_{gwl} - \phi_{drain,i}}{\gamma_{drain,i}}, \quad (8)$$

where $q_{drain,i}$ represents the drainage/infiltration (cm d⁻¹) to and from the surface water system i , the drainage base $\phi_{drain,i}$ is equal to the surface water level of the system i (cm below the soil surface), ϕ_{gwl} is the groundwater level (cm below the soil surface), and $\gamma_{drain,i}$ is the drainage or infiltration resistance of the system i (d).

2.3. Model coupling approach

Due to the rapid fluctuations of vadose zone water dynamics and slow movement of groundwater flow, the groundwater modeling always has larger spatial and temporal scales than vadose zone modeling. Moreover, solving the non-linear Richards equation (Eq. (2)) often requires much shorter time steps compared to solving the groundwater flow equation (Eq. (1)). Thus, to couple the vadose water flow processes with groundwater flow models, one challenge is to deal with these different temporal and spatial scale problems. Fig. 2 depicts the conceptualization of the coupled model development, using three simulation units and three corre-

sponding SWAP zones as an example. In MODFLOW, the modeling domain was discretized into a 3-D finite-difference grid. The flux components, including the vertical net recharge from the soil profile, groundwater abstraction, drainage, river recharge, leakage, etc., were imposed on the grid cells to solve the finite-difference approximation of mass conservation equation. The SWAP zones were defined to represent a homogeneous sub-region of the vadose zone processes, and were specified to the corresponding MODFLOW grid. Each SWAP zone consists of one or more cells of MODFLOW grid (Fig. 2). It is feasible to define the SWAP zones on a cellwise basis, however, it is not always necessary for most practical situations because of the very complicated data processing and large computation. The soil profile for each SWAP zone was vertically discretized into a 1-D finite-difference grid, whose thickness was much smaller than the vertical layer thickness of the MODFLOW grid.

A disparity exists with respect to temporal scales of vadose zone flow and groundwater flow. To deal with this issue, different time steps were used to solve the vadose zone flow and groundwater flow in the coupled model. Each MODFLOW time step consists of many SWAP time steps. As shown in Fig. 3, the vadose zone and groundwater flow models are interactive through the exchange of averaged water table depth and vertical net recharge flux and the calculated specific yield S_y if needed in each MODFLOW time step. The initial hydraulic heads of MODFLOW were used to calculate the averaged water table depth for each SWAP zone at the first MODFLOW time step of the first stress period. Initially, the bottom flux at the soil profile of each SWAP zone was calculated by the SWAP package, and was subsequently specified to the corresponding SWAP zone as a net recharge flux at start of each MODFLOW time step. The S_y value for phreatic aquifers is affected by soil water retention properties, water table depth and its change rate, etc. (Sophocleous, 1985), especially under shallow water table conditions. In the coupled model, three options were provided to determine the values of S_y when using the SWAP package. The values of S_y can be specified directly by users as a constant according to the results of pumping or slug test. The S_y value can also be calculated for each SWAP zone at start of each new MODFLOW time step by using Eq. (9) (Stoppelenburg et al., 2005) or Eq. (10) (Duke, 1972; Said et al., 2005):

$$S_y = \frac{\sum_{i=1}^k (\theta_s - \theta) DZ_i}{\sum_{i=1}^k DZ_i}, \quad (9)$$

$$S_y = (\phi - S_r) [1 - (h_a / GWTD)^\tau], \quad (10)$$

where DZ_i is the thickness of the i th soil compartment (cm) and k is the total number of soil compartments above the water table; ϕ is the porosity (cm³ cm⁻³), S_r is the soil specific retention (cm³ cm⁻³), τ and h_a are the pore size distribution index and the soil air entry pressure (cm) of Brooks and Corey water retention model (Brooks and Corey, 1966), respectively, and $GWTD$ is the depth to water table (cm). The updated averaged water table depth for each SWAP zone was calculated by MODFLOW, and assigned to SWAP zones in order to determine the hydraulic head at the bottom of the soil profile for the next MODFLOW time step using Eq. (7). This coupled model ran iteratively through the exchange of the averaged water table depth and the net recharge flux in SWAP zones for each MODFLOW time step, as shown in Fig. 3. However, if the water table becomes lower than the bottom elevation of the soil profile, the bottom boundary will be switched into a free drainage condition for the corresponding SWAP zone. The net recharge to water table can be optionally specified to the cells of the first layer or the upper active cells of MODFLOW by users.

Any length of time step can be selected by users as needed in MODFLOW. However, a 1-day time step was used for MODFLOW

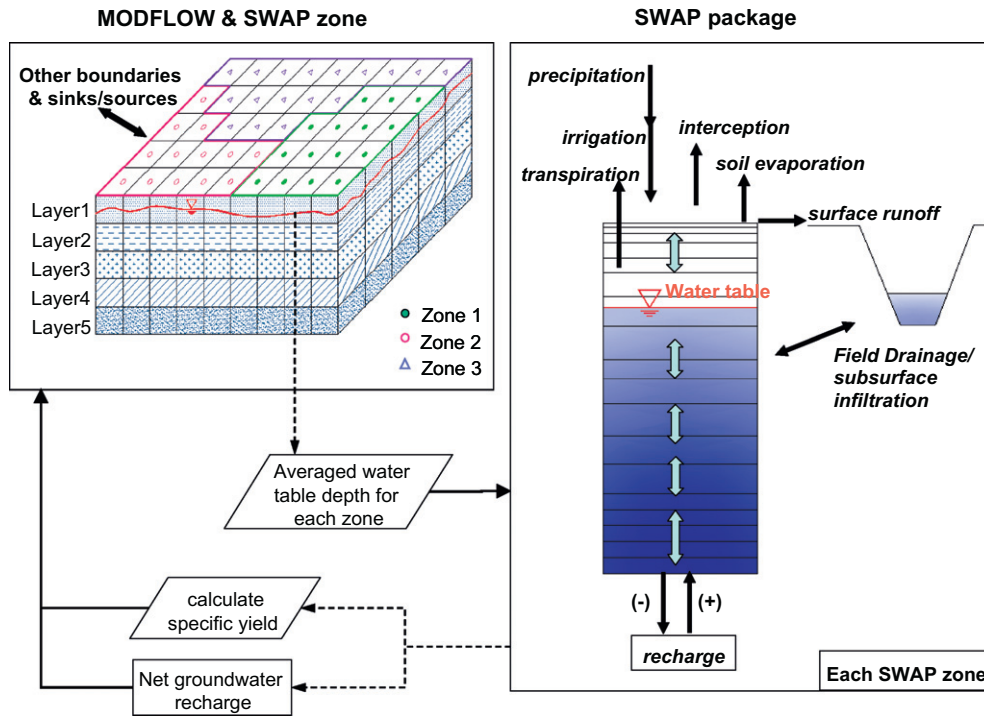


Fig. 2. Schematic diagram of the MODFLOW-2000 model and its coupling with the SWAP package, showing the data exchange procedure using three SWAP zones as an example.

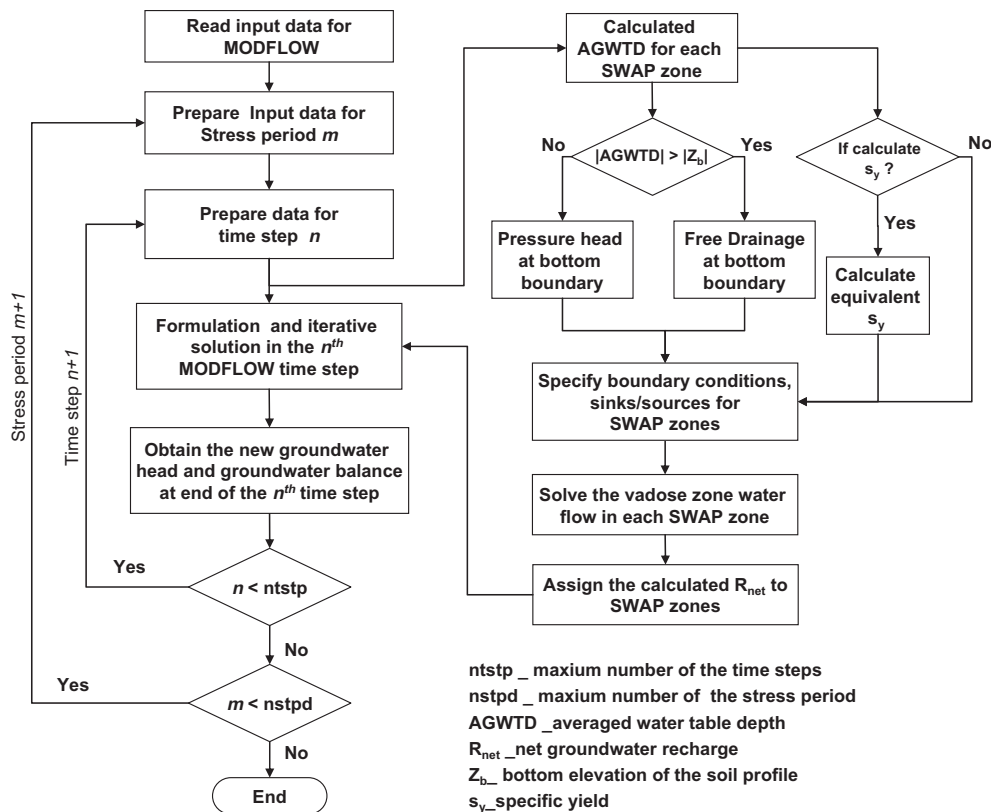


Fig. 3. The calculation procedure of the MODFLOW-2000 with the SWAP package.

if Penman–Monteith equation was chosen for calculating ET_p because this equation is based on a daily calculation in the SWAP package.

The results of the vadose zone flow and groundwater flow were saved separately. MODFLOW-2000 reported the groundwater head and groundwater balance at the end of a user-specified time step.

Meanwhile, SWAP provided the moisture information of the soil profile for specified time. In this study, we have the option of using the SWAP package to replace the RCH-EVT or RCH-ETS packages of MODFLOW. However, for those sub-regions without enough soil information to use the SWAP package, the RCH, EVT or ETS packages of MODFLOW can still be simultaneously used with the SWAP package. RCH package is also needed to simulate recharge in SWAP zones from other sinks or sources besides of the groundwater recharge and evapotranspiration through the vadose zone. Such kinds of flexibility make this coupled model friendly to users for various applications.

3. Test study

3.1. Case study 1: 2-D water table recharge experiment

3.1.1. 2-D water table recharge experiment

Due to the lack of analytical solutions to such a coupled system, a 2-D water table recharge experiment, presented in detail by Vauclin et al. (1979), was chosen to test the applicability of the SWAP package. The dataset of this experiment has been widely used to test the variably saturated flow models (Clement et al., 1994), or the coupled saturated–unsaturated models with simplified treatment of the unsaturated flow process (Thoms et al., 2006; Shen and Phanikumar, 2010; Twarakavi et al., 2008). The flow domain consists of a rectangular sandy soil slab of 6.0 m long, 2 m high and 0.05 m thick. The bottom of domain can be defined as the reference datum and the initial pressure head is 0.65 m above the domain bottom. At the soil surface, a constant flux of $q = 3.55 \text{ m d}^{-1}$ was applied to over the central 1.0 m by 0.05 m area, while the rest soil surface was covered to prevent soil evaporation. Because of the symmetry of the flow system, only flow in one half of domain (right side) with size of $3.0 \text{ m} \times 2.0 \text{ m}$ needs to be modeled (Fig. 4). The setup of the coordinate system is shown in Fig. 4. No-flow boundaries were defined on the bottom and the left side of the modeled domain (water divide due to the symmetry of flow). The water table elevation on the right boundary of the flow domain is 0.65 m throughout the entire experiment. The soil hydraulic properties were obtained from Vauclin et al. (1979), and the parameter values for van Genuchten model are presented in Table 1 (Thoms et al., 2006).

3.1.2. Model setup

In the simulation with MODFLOW, the flow domain was divided into 1 row, 30 columns and 1 layer. The grid was horizontally

discretized into uniform rectangular cells of 5 cm height and 10 cm width, and the thickness of the layer was assigned to 200 cm. It was assumed that the domain is homogeneous and isotropic. The hydrogeological parameters were obtained from Vauclin et al. (1979). The hydraulic conductivity of 840 cm d^{-1} was used, and the value of S_y was calculated using Eq. (9) in each MODFLOW time step.

The simulation period lasted 8 h with one stress period and the time step of 2 min. The bottom of domain was used as the reference datum in MODFLOW. The initial hydraulic heads are 65 cm for all cells. The SWAP package was used to define the upper boundary conditions. Eleven SWAP zones were defined considering the recharge zones (zones 2 and 3) and non-recharge zones (zones 4–11) (Fig. 4), while zone 1 was used to define the zone with zero net recharge. The right side of flow domain was assigned as a 65 cm constant-head boundary. No-flow boundaries were defined on the bottom and the left side of the modeled domain in MODFLOW (Fig. 4).

With the SWAP package, identical homogeneous soil profile was considered for all SWAP zones with the same values of van Genuchten parameters as shown in Table 1. The recharge flux was simulated as the precipitation since the reference evapotranspiration rate was assigned to zero. The bottom boundary (i.e., the hydraulic head at the bottom of the soil profile) was determined using the averaged water table depth of corresponding SWAP zone. The initial conditions of soil moisture were assigned to each compartment of soil profile according to the measurements of Vauclin et al. (1979).

3.1.3. Simulation results

The simulated water table using MODFLOW-2000 with the SWAP package was compared with the measured water table as shown in Fig. 5. It was found that the simulated water tables at 3, 4 and 8 h matched well with the observed water tables; however, the model obviously overestimates the water table at 2 h. This overestimation may result from that the model does not accounts for the horizontal water flow in the unsaturated zone, which can be significant during the early period due to the relatively low initial soil moisture close to land surface. Lateral moisture diffusion caused the inflow from recharge zone to be redistributed horizontally in the vadose zone before it reached the water table, and the unsaturated zone can store a portion of the inflow. However, our model assumes that lateral redistribution of water occurs only after water has entered into the saturated zone. Therefore, our model overestimated the net groundwater

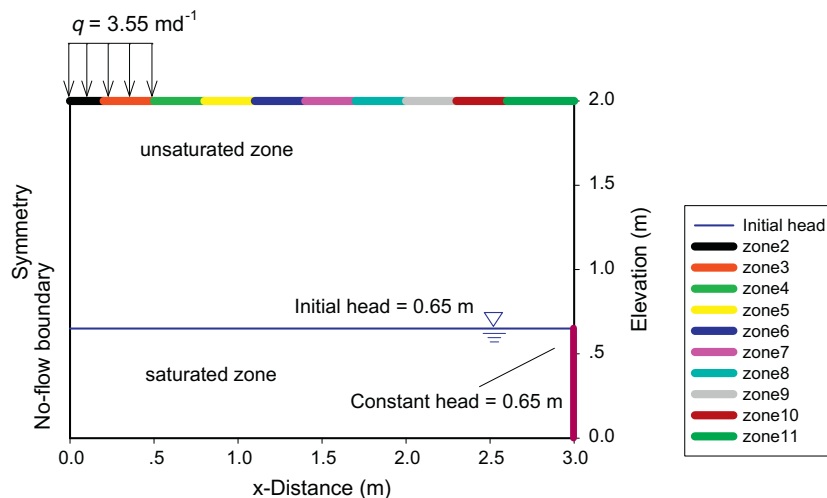


Fig. 4. Description of a 2-D variably saturated water table recharge experiment (Vauclin et al., 1979) and its modeling setup using MODFLOW with SWAP package.

Table 1
Values of the Mualem–van Genuchten model parameters in Eqs. (3) and (4).

Soil	Layer thickness (cm)	θ_s (cm ³ cm ⁻³)	θ_r (cm ³ cm ⁻³)	α (cm ⁻¹)	n (-)	λ (-)	K_s (cm d ⁻¹)
Fine river sand	200	0.30	0.0099	0.033	4.1	0.5	840

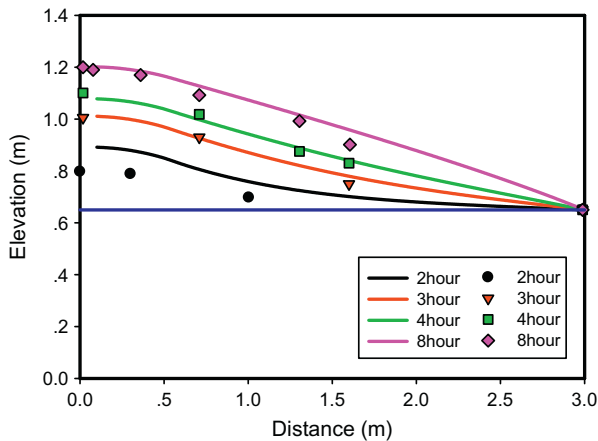


Fig. 5. Comparison of observed and simulated water table elevations at 2, 3, 4 and 8 h in the experiment.

recharge and subsequently resulted in a higher water table at the early stage for this particularly test problem, as also evident in Fig. 5. However, as the water table rose, more groundwater will be drained out through the constant head on the right side. The flow system then gradually approached to the steady-state condition. Subsequently, the simulated water tables agreed well with the observed ones at 3, 4 and 8 h. Especially at 8 h, the simulated and observed water tables were in a good agreement. These phenomena are quite similar to the result obtained by Shen and Phanikumar (2010).

The observed and simulated distributions of soil water content in soil profile for initial and 8 h are presented in Fig. 6. The simulated and observed soil water content agreed well at $x = 20$ cm where the vertical flow was dominant in the unsaturated zones. But neglect of lateral moisture diffusion may result in a slightly higher simulated water moisture than the observed one at 8 h (Fig. 6a). Much closer agreements were observed at $x = 140$ and 200 cm where the lateral water flows were so small and nearly negligible, which may be due to that this region was away from the recharge area ($x = 0$ –50 cm) (Fig. 6d and e). However, the simulated water moisture was apparently lower than the observed one in the unsaturated zone at locations of $x = 60$ and 80 cm, which was closer to the recharge area of ($x = 0$ –50 cm) (Fig. 6b and c). It was known that the effect of lateral diffusion effect in vadose zone may be weaker in actual regional flow problems compared to this experiment, and the vadose zone water flow can be assumed to mainly occur in the vertical direction for many irrigated areas such as described by Singh et al. (2006) and Droogers et al. (2000). Therefore, the coupled model in this study may result in less error due to the ignorance of later diffusion effect for most of the practical problems.

3.2. Case study 2: Regional groundwater flow simulation

3.2.1. Study area

In order to verify the proposed MODFLOW with SWAP package for real applications on a regional scale, the Yonglian Irrigation System (YLIS) of Hetao Irrigation District (Hetao) in North China was selected as a study area in this case (Fig. 7). It has a typically arid continental climate with shallow water tables caused by improper

agricultural irrigation practices. The mean annual precipitation is only 169 mm, with most of the rainfall occurring from July to September in the YLIS. The mean annual temperature is 6 °C, with the lowest and highest monthly averages being –13 °C and 22 °C in January and July, respectively. The mean annual evaporation is about 2000 mm. Soils in the southern part include alluvial silt sediments with textures of sandy loam types, while in the northern part they are finely textured, such as silt loam or clay loam.

The YLIS is located east of the Naiyong sub-main drainage ditch and west of the Yongshen sub-main drainage ditch (see Fig. 7). It is bounded by the sixth sub-main drainage ditch in the north, and by the south part of Yongshen sub-main drainage ditch and the upper reaches of the Zaohuo sub-main canal on the south border. The topography is flat, with a gradient of 1/4000 from south to north.

Due to the special climatic condition in the region, irrigation is essential during the entire crop growing season. All irrigation water is diverted from the Yellow River, while surface basin irrigation remains the major irrigation method. Canal seepage and field percolation cause a high water table in Hetao. Subsequently, the amount of groundwater evapotranspiration is very large, which results in severe problems of soil secondary saline-alkalization (IWC-IM, 1999).

The aquifer geometry and hydrogeological parameter data were obtained from boreholes and pumping tests (Wu, 2007; IWC-IM, 1999). This region is underlain by Quaternary sediments, mainly lake sediments and alluvial deposits from the Yellow River. The unconfined aquifer is composed of two water-bearing strata (Q4 and Q3) with respective thicknesses of 5–7 m and 39–45 m. The Q4 stratum is mainly sandy loam, and becomes finer from south to north, while the Q3 stratum consists of fine-medium sand, fine sand and silt sand with clay inter-layers. The Q4 stratum has a lower permeability and the Q3 stratum has a relatively high permeability. The upper layer of Q2 (Q₂¹), located below the Q3 and Q4, is stable muddy clay, acting as a low permeable aquitard (Wu, 2007; IWC-IM, 1999).

The flow of groundwater moves from south to north according to hydraulic head measurements at 10 observation wells (see Fig. 7). Hydrogeologists from the Hetao Administration Office monitor the water table manually once every 5 days. The hydraulic gradient of the water table is about 1/3000–1/5000, which is approximately the same as the topographic slope (IWC-IM, 1999).

3.2.2. Model setup

The data sets used for model construction in this section were primarily obtained from several previous studies (Wu, 2007; IWC-IM, 1999; Bameng Survey, 1994) and from field survey. The aquifer system was divided into two sub-aquifers, with the first sub-aquifer on top of the second sub-aquifer. The first sub-aquifer has one layer. The second sub-aquifer was assumed to have uniform hydrogeological parameter values and was divided into three layers with uniform thickness, due to the relatively larger thickness compared to the first layer. Thus, the aquifer system was vertically discretized into four layers. A uniform rectangular grid with 100 m square cells was used. The first layer, representing the Q4 stratum, is a low-permeable layer with a thickness of 5–7 m, while layers 2–4 consist of Q3 stratum and have higher permeability, with thicknesses varying from 13 to 15 m from south to north.

It is assumed that the aquifer is horizontally isotropic with its horizontal hydraulic conductivity being five times larger than the vertical one. The hydrogeological parameters were available from

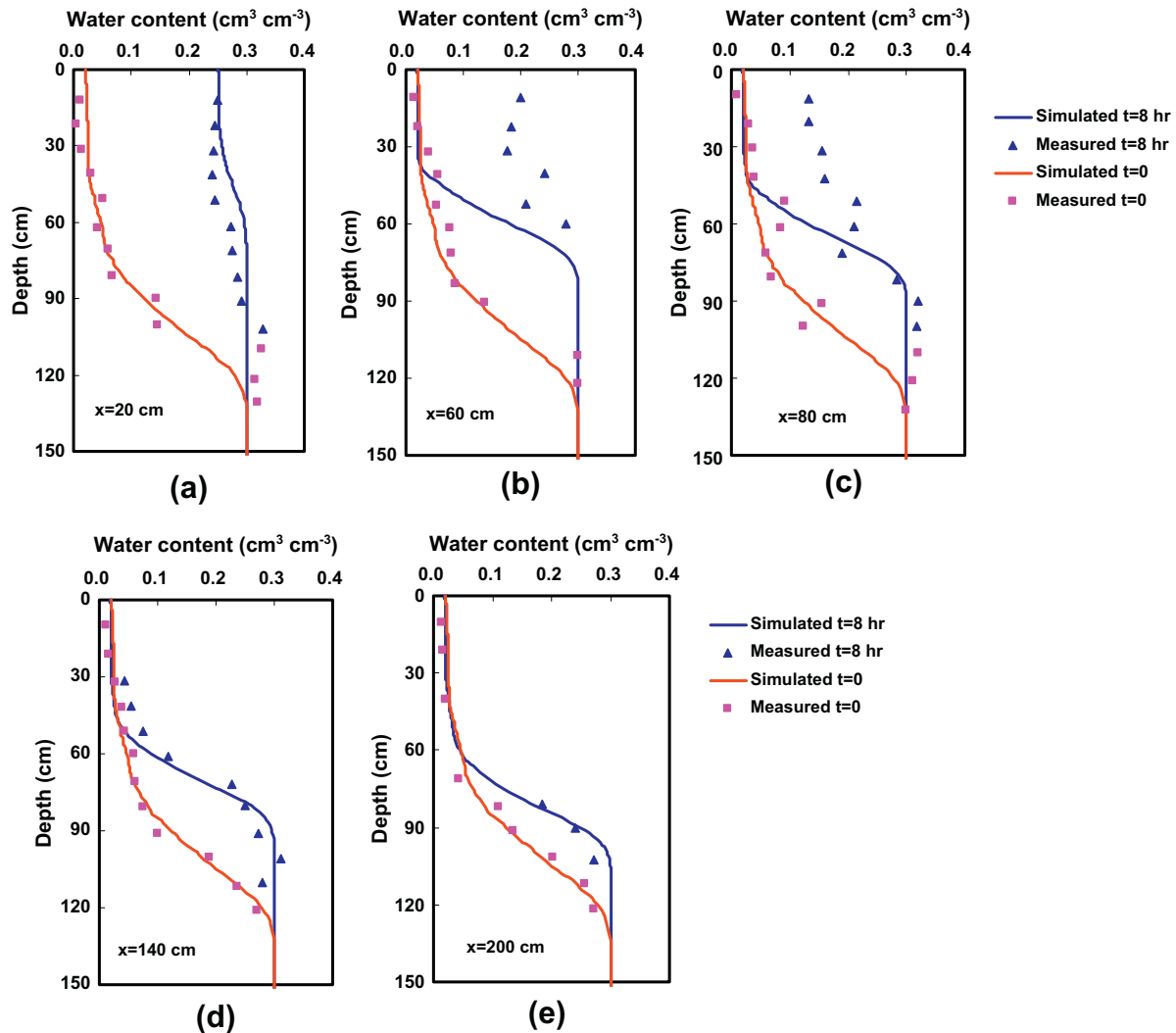


Fig. 6. Comparison of soil moisture distribution in the soil profile at different locations: (a) $x = 20$ cm; (b) $x = 60$ cm; (c) $x = 80$ cm; (d) $x = 140$ cm; (e) $x = 200$ cm.

the previous studies (Wu, 2007; IWC-IM, 1999). The horizontal hydraulic conductivity for the first layer varies between 0.6 and 1.0 m d^{-1} in the north–south (N–S) direction. The value of S_y was estimated using Eq. (10) for the phreatic aquifer – layer 1. The values of $(\phi - S_r)$, τ , h_a are respectively equal to 0.09, 0.43, 23 cm for south area with sandy loam and 0.084, 0.39, 25 cm for north area with loam soil. Layers 2–4 have the same hydraulic conductivity, which range from 8 to 10 m d^{-1} along the N–S direction; their corresponding S_y equals to 0.20 and their specific storage is 10^{-6} m^{-1} . The simulation period lasted from May 1, 2004 to October 31, 2004 with 1-day time step. Initial groundwater heads were obtained through interpolation of observed groundwater levels from 10 wells on May 1, 2004.

The drainage ditches were considered as drain boundaries using the Drainage (DRN) package in MODFLOW for the first layer on the north, west and east borders. In the south, the upper part of the Yongshen sub-main drainage ditch and the upper reaches of the Zaohuo canal were simulated using a drain boundary and a flux boundary for the first layer, respectively. No-flow boundary conditions were defined for the lower layers. The recharge due to canal seepage was a calculated average, assigned to the canal control region, and computed with the RCH Package in MODFLOW.

Nineteen SWAP zones were defined for the study area through the combination of soil type, land use, irrigation system and depth

to water table for vadose zone flow modeling (Fig. 8). Two soil types including sandy loam and loam were considered, corresponding to zones 2–8 in the south and zones 9–19 in the north, respectively. These two soil types were represented by two soil profiles with a thickness of 3 m for each. The soil profiles were divided into three horizontal layers and forty compartments in the SWAP modeling. The values of Mualem–van Genuchten model parameters (see in Table 2) for the horizontal layers of two soil profiles were determined according to previous studies (Wu, 2007).

The crops cultivated in the study area were simplified into two main crops: summer maize and sunflower. Maize grew in the south area (zones 2–8), while sunflower growth was in the north area (zones 9–19) (Fig. 8). The crop growth data, including development stage, leaf area, crop height and root depth were collected from Wu (2007). Other parameters required by the simple crop module were assigned according to Kroes and van Dam (2003).

The weather data obtained from the nearby Hangjinhouqi County weather station was used for simulation. The rainfall was obtained from the rain gauge measurements in the YLIS. The basic drainage module was used and its parameters were obtained from Wu (2007). The bottom boundary (i.e., the hydraulic head at the bottom of the soil profile) was determined using the water table depth.

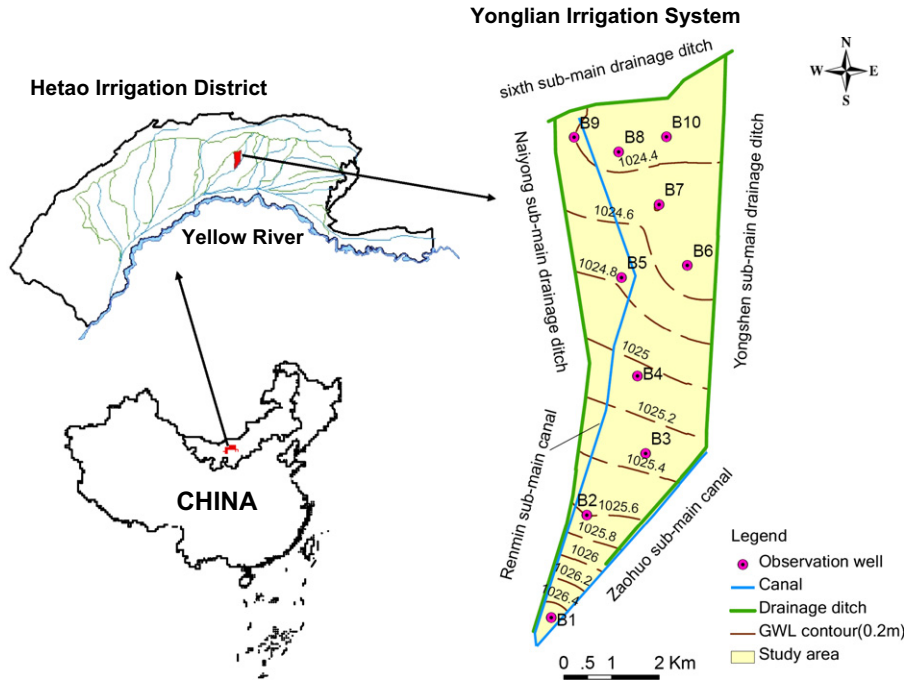


Fig. 7. Yonglian Irrigation System, locations of the observation wells, and contour map of the initial groundwater level (GWL).

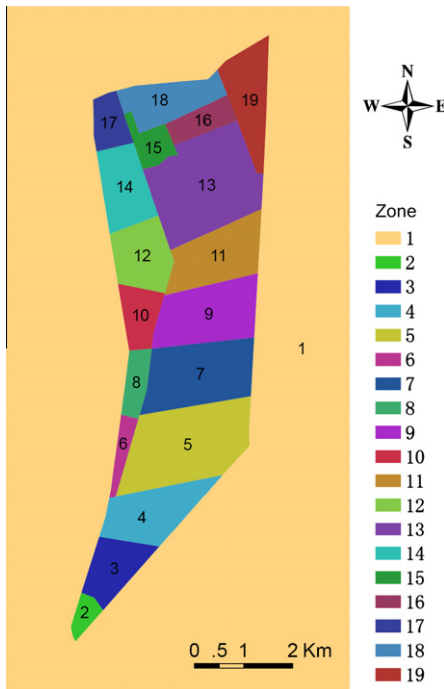


Fig. 8. The definition of SWAP zones in the study area (zone 1 represents the inactive cells of the flow domain).

3.2.3. Simulation results

Groundwater level data from 10 observation wells (Fig. 7) were used to evaluate the model performance. The root mean square error (RMSE) and the model efficiency (EFF) were used as indicators of model fitting:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (GW_i^{obs} - GW_i^{sim})^2}, \tag{11}$$

$$EFF = 1 - \left[\frac{\sum_{i=1}^n (GW_i^{obs} - GW_i^{sim})^2}{\sum_{i=1}^n (GW_i^{obs} - GW^{mean})^2} \right], \tag{12}$$

where GW_i^{obs} and GW_i^{sim} are respectively the i th value of the observed and calculated water table ($i = 1, 2, \dots, n$), n is the total number of observations, and GW^{mean} is the average observed water table over the total number of observations. Good agreements between measured and simulated groundwater levels were achieved for the 10 selected observation wells (Fig. 9). The RMSE and EFF of groundwater level for a 5-day observation interval were 0.23 m and 0.93, respectively. Fig. 9 also shows that the simulated groundwater level agrees well with the observation. The observed and simulated groundwater levels were compared through a linear regression forced to the origin, and the respective coefficients of regression and determination were $b = 1.0$ and $R^2 = 0.93$. The simulated daily groundwater levels of four observation wells (B3, B4, B5 and B8) are selected and presented in Fig. 10. The observation wells B3&B4 and B5&B8 were respectively located in the south area with sandy loam and in the north area with loam soil. It showed that fluctuations of simulated groundwater levels agreed reasonably with the observation data. However, some discrepancy still exist between the simulated groundwater levels and the observations, e.g., the simulated groundwater levels at observation well B3 show slightly lower than the observed ones, while the simulated groundwater levels at B5 are higher than observed ones in June. This implies that uncertainties may be imposed by model parameters, model structure and model input.

The MODFLOW with SWAP package gave a reasonable description of water table fluctuations responding to rainfall, irrigation and evapotranspiration, compared to artificially-designated recharge or discharge rates, as shown in Fig. 10. The groundwater level rose quickly after irrigation or rainfall, and declined due to direct evaporation and crop root uptake during May to late July. A continuous declining trend was observed due to direct evaporation and crop root uptake and less irrigation or rainfall from early August to late September (Fig. 11). The water table depth decreased from 0.6–1.0 m to more than 2.0 m during the same period. In October,

Table 2
Values of the Mualem–van Genuchten model parameters for two soil types in the Yonglian Irrigation System, North China.

Soil types	Layer (thickness)	θ_s (cm ³ cm ⁻³)	θ_r (cm ³ cm ⁻³)	α (cm ⁻¹)	n (-)	λ (-)	K_s (cm d ⁻¹)
Type 1	Loam (0–40 cm)	0.42	0.02	0.013	1.6	0.5	15.1
	Sandy loam (40–150 cm)	0.41	0.02	0.014	1.32	0.5	17.4
	Loam (150–300 cm)	0.45	0.01	0.048	1.36	0.5	14.3
Type 2	Loam (0–40 cm)	0.43	0.02	0.0104	1.44	0.5	11.13
	Clay loam (40–150 cm)	0.46	0.02	0.0096	1.32	0.5	12.2
	Silt loam (150–300 cm)	0.45	0.01	0.0117	1.33	0.5	13.3

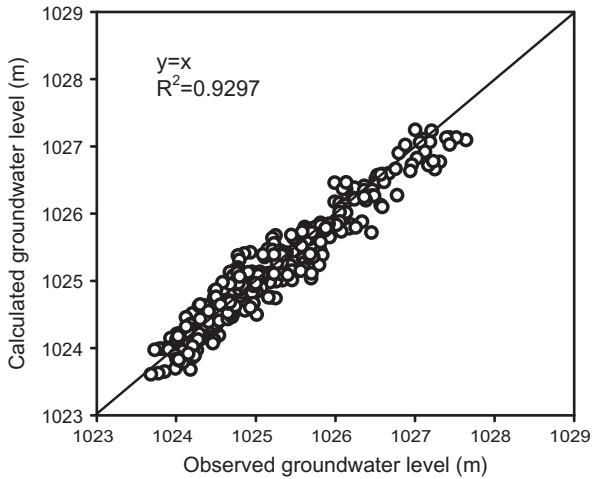


Fig. 9. Comparison of the observed and calculated groundwater levels for 10 observation wells (Fig. 7).

the water table increased markedly, a result of the prescribed autumn irrigation process for leaching salt and storing water in the soil profile for crop use for the next agricultural year.

The value of actual evapotranspiration (ET_a) in vadose zone was in a range of 453–536 mm from May 1st to September 20th for all SWAP zones, which is close to the results of Wu (2007) with a water balance method in YLIS. The temporal variation of ET_a and net bottom flux (Q_{bot}) in SWAP zone 13 is presented in Fig. 11. A positive Q_{bot} represents upward groundwater flow to recharge the vadose zone, and a negative Q_{bot} means downward flow to recharge groundwater from the vadose zone. Result showed that groundwater recharge was closely related to the irrigation and rainfall, while large groundwater capillary rise was contributed to crop water use during the crop growing period from June to middle August. Those imply the coupled model can reasonably reproduce the flow pattern in vadose zone.

4. Discussion

The two case studies showed that the coupled model can reasonably simulate groundwater and vadose zone water dynamics

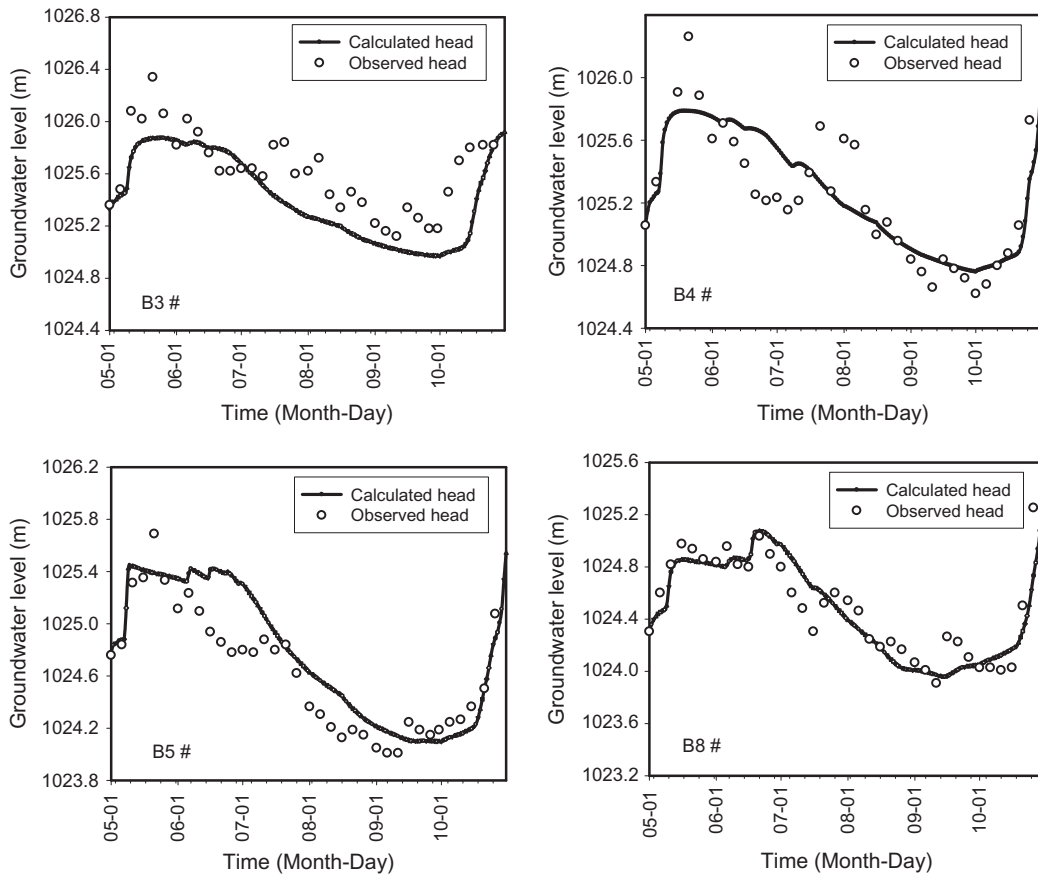


Fig. 10. Comparison of the observed and calculated groundwater levels for the four selected observation wells (B3, B4, B5, B8).

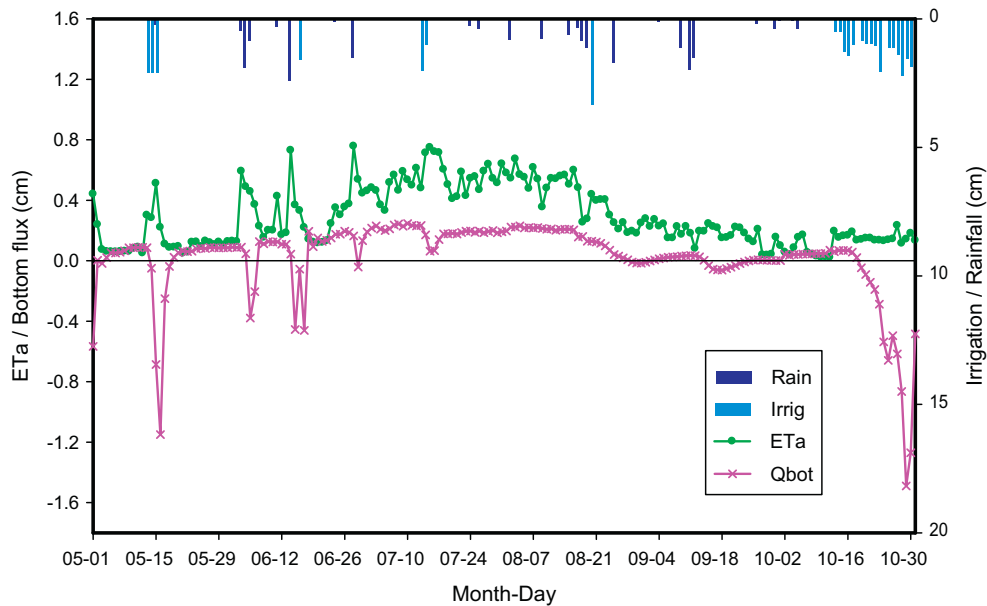


Fig. 11. Actual evapotranspiration (ET_a) and vertical bottom flux (Q_{bot}) versus rainfall (*Rain*) and irrigation (*Irrig*) in zone 13.

under the conditions that the vertical water flow is dominant in vadose zone. The coupled model simulation can help us gain greater insights into the spatial and temporal pattern of groundwater recharge and evapotranspiration, and fluctuation of water tables accounting for the spatial and temporal variations of topography, soil, land use and water management practices on a regional scale. However, in spite of these favorable advantages, it is necessary to know its limitations and improvements needed when using the SWAP package. Firstly, the current version of SWAP package does not take into account the effects of terrain changes (i.e., slope and aspect) on surface water movement and its interaction among SWAP zones. Therefore, it is not applicable for the regions with strong surface runoff such as hilly and mountain regions in humid and semi-humid regions. This may be solved by employing the concept of rainfall-runoff mode as used in the Soil and Water Assessment Tool (SWAT) model (Arnold et al., 1993) in further investigation. Secondly, the solute transport has not been employed at this study. Thus, the current version of SWAP package is not suitable for regions which have severe salinization problems. In those regions, vegetation growth will be seriously affected by solute transport processes, which will significantly affect groundwater recharge and evapotranspiration pattern. Waterlogged areas in arid and semi-arid regions often have the salinization problems or the potential threat to become salinization over time (Petheram et al., 2003). Thus, integrating a solute transport module both for vadose zone and saturated zone such as MT3D (Zheng, 1990) into our developed model will be a follow-up subject to investigate. Thirdly, for regions with deep water tables (thick vadose zones), it is increasingly difficult to characterize the hydrological properties of the unsaturated zones because of the heterogeneous nature of the media, which will make our model less reliable. Finally, the SWAP package of coupled model is more suitable for the areas with relatively small changes in depth to water table in space. Otherwise, a finer discretization is needed for local regions with greatly spatial variations of depth to water table, which may impound heavily on available computational resources or bring some uncertainties. An alternative method is to use RCH-ETS packages instead of SWAP package for estimating recharge and evapotranspiration in local regions with highly spatial variations of depth to water table.

5. Summary and conclusion

We have presented the development of a SWAP package for the MODFLOW-2000 model to simulate the vadose zone flow processes and estimate the groundwater recharge and evapotranspiration for groundwater modeling in relation to the shallow water problems. The SWAP package was simplified from the original SWAP model by only considering the flow process and neglecting the solute and heat transport processes. This simplified SWAP package was adapted to describe the vertically 1-D vadose zone water movement. It considered the effects of infiltration, soil evaporation, crop root uptake, soil moisture storage, drainage in field scale, crop growth, and surface runoff in the vadose zone. Therefore, it includes most important processes related to groundwater recharge and evapotranspiration estimation. The MODFLOW-2000 model was used to simulate three-dimensional groundwater flow, interacting with the SWAP package through an exchange of net recharge flux and averaged water table depth in each SWAP zone. The MODFLOW-2000 coupled with the SWAP package was then tested using a two-dimensional saturated-unsaturated water table recharge experiment of Vauclin et al. (1979) and a regional groundwater flow simulation in an arid irrigation district of North China. The agreement of simulated and observed water table validates the practical applicability of this coupled model. Finally, the limitation and improvement needed for the current version of the coupled model were analyzed. This calls for a follow-up investigation on integration of the solute transport, surface water movement to the current model as well as a combination with the remote sensing technologies.

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