Case study

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Coupling of WetSpass-M and MODFLOW models for groundwater flow assessment

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Abstract: Recharge is considered a key parameter in groundwater models for sustainable management of aquifers, which is influenced by factors such as land use, soil and weather. The present study was conducted to couple WetSpass-M and MODFLOW models in the Neyshabur–Rokh Basin. To this aim, the simulated recharge by the WetSpass-M model was applied as an input into MODFLOW to assess the groundwater balance. The hydrodynamic coefficients were determined by calibrating the model, and the model sensitivity to the hydraulic conductivity coefficient, specific yield and recharge was evaluated. The results indicated that the annual average of surface runoff, actual evapotranspiration, interception and recharge during 1991–2017 equalled 18, 36, 7.6 and 42.6% of the average annual precipitation in the basin, respectively. The accurate alignment of simulated and observed water levels, along with the achievement of suitable evaluation criteria values in both steady and transient states, demonstrates the WetSpass-M model's precision in estimating recharge and successfully integrating the two models. The groundwater balance assessment revealed a significant deficit in the aquifer, with the model demonstrating greater sensitivity to the hydraulic conductivity coefficient and providing valuable insights for the sustainable management of the Neyshabur aquifer.

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Groundwater has emerged as a strategic resource not only in most arid and semi-arid countries but also in humid climates over the last 50 years (Shah 2014). The high quality and relatively stable state of such waters compared to surface ones are among the reasons for increasing the use of groundwater (Siebert *et al.* 2010). Approximately 750–800 billion cubic metres (BCM) of groundwater are consumed in agriculture on a global scale (Shah 2014). Groundwater is regarded as a basic source of fresh water for humans, which constitutes more than 70% of water supply sources in arid and semi-arid regions. These resources have been reduced due to overharvesting for irrigated agriculture at local and regional scales during recent decades. In addition, the significance of groundwater resources is predicted to increase in dry areas, including Iran, due to future climate changes, periods of drought and reduced access to surface resources (Hashemi *et al.* 2015). Groundwater is considered a strategic and necessary source all over the world for all of the aforementioned reasons. Thus, the effective management of such resources is regarded as a critical and urgent challenge. In addition, sustainable management of groundwater requires acquiring enough knowledge regarding recharge (Tilahun and Merkel 2009). Therefore, determining the amount of groundwater recharge is considered as a prerequisite for efficient and sustainable management of such resources since the amount of withdrawal from the groundwater in a region in the long term should not be higher than the long-term average of its recharge. Thus, estimating the recharge determines the appropriate level of groundwater extraction (de Vries and Simmers 2002).

Groundwater models are often applied to simulate water flow in aquifers. Such models can be used to simulate the long-term behaviour of an aquifer under different management plans when they are calibrated. Recharge is regarded as a critical parameter in groundwater models. Despite its strengths, this model has some limitations that need to be considered. One of the main limitations is the lack of properly estimated recharge and its spatio-temporal distribution, which make these models unreliable (Sophocleous 2005).

The direct recharge of groundwater due to precipitation is often included in the model as a percentage of the aquifer rainfall in arid and semi-arid regions (Hashemi *et al.* 2015), while groundwater recharge exhibits a random behaviour (Sen 2008), which is influenced by factors such as weather conditions, variety of land use, soil, and vegetated cover temporally and spatially (Kim *et al.* 2008). In this study, the monthly water balance of the WetSpass-M (Water and Energy Transfer between Soil, Plants and Atmosphere under quasi-Steady State-Monthly) distributed hydrological model (Abdollahi *et al.* 2017) was utilized to estimate the groundwater recharge as the mentioned factors cannot be considered in groundwater models, and the WetSpass-M water balance distribution model can regard the above-mentioned factors and has shown acceptable performance as a successful instrument in estimating the spatio-temporal distribution of recharge in previous studies (Shrestha *et al.* 2016; Kahsay *et al.* 2018; Salem *et al.* 2019; Ashaolu *et al.* 2020; Gelebo *et al.* 2022; Yenehun *et al.* 2022). The groundwater flow was then simulated in steady and transient states with the entry of WetSpass-M recharge to the MODFLOW. Such a method is applied in the Neyshabur watershed as one of the potential agricultural basins in the Razavi Khorasan province of Iran. The Ministry of Energy has designated this area as a critically restricted zone since 1987 due to the excessive exploitation and significant depletion of groundwater resources, as well as the emergence of a negative balance.

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Few studies have been conducted on spatio-temporal estimation of groundwater recharge using the WetSpass-M model and its evaluation in the groundwater balance. Aslam *et al.* (2022) examined the WetSpass-M and MODFLOW models to investigate the effects of recharge and discharge on the Chaj Doab aquifer in the Punjab region of Pakistan. Values of evaluation criteria – root mean square error (RMSE) = 0.0022, mean absolute error (MAE) = 0.5158 and mean error (ME) = 0.01836 – during the calibration period of the MODFLOW model in the transient state indicate the success of utilizing the estimated recharge by WetSpass-M in the groundwater model. In the next step, three management scenarios were considered in order to predict the future state of the aquifer. The continuation of pumping from 2003–19 until 2035 will lead to an 18.1 m decrease in the groundwater level. The above-mentioned scenario predicts the most serious of the three management scarios for the aquifer. Ghouili *et al.* (2017) utilized the WetSpass model to assess the groundwater recharge values for the Takelsa multilayered aquifer in Tunisia across seasonal and annual timescales. Subsequently, they employed the MODFLOW model to simulate groundwater flow in a steady state. The study's findings revealed how surface runoff, recharge and evapotranspiration formed from rain.

Considering the significance of recharge and its fundamental role in groundwater aquifers, the WetSpass-M and MODFLOW models were synchronized to achieve the following general scientific objectives: (1) an estimation of the spatial distribution of water balance components in the Neyshabur watershed in monthly time steps during 1991–2017; (2) an evaluation of the performance of the estimated recharge using the WetSpass-M model to simulate the aquifer conditions in steady and transient states in the groundwater flow model; and (3) determination of the hydrodynamic coefficients of the aquifer. In comparison to previous studies, this research represents the first attempt to estimate recharge using WetSpass-M in the Neyshabur–Rokh Basin on a monthly scale.

Determining the water balance and knowing the characteristics of the Neyshabur watershed and aquifer can be a fundamental step in providing appropriate solutions to eliminate obstacles in such a critical agricultural basin in the Razavi Khorasan province and to compensate for its aquifer deficit.

Materials and methods

Study area

The Neyshabur watershed is regarded as including part of the Kavir-e Markazi Basin in Iran and part of the Kal Shur watershed, located between 58° 13′ and 59° 30′ E longitude, and between 35° 40′ and 36° 39′ N latitude, and is in the centre of the Razavi Khorasan province. Of a total area of 9449 km^2, the aquifer of the basin occupies 2883.4 km^2. The average slope of the watershed is 6.86%, the altitude of the study area is between 1056 and 3309 m, and its lowest point is located at the outlet of the aquifer, namely the Hosseinabad Jangal region. As the average annual precipitation and evaporation of this basin are 246.86 and 2357.23 mm, respectively, and its annual average temperature is 13.3°C, in terms of climatic conditions it is classified as a semi-arid to arid region. The network of surface streams flows towards the centre of the plain from the northern, northwestern, eastern and southern elevations in the form of permanent rivers and various intermittent streams, after joining the Kal Shur as the main drain rerouted to the west and exiting from the outlet of the study area. The study area is

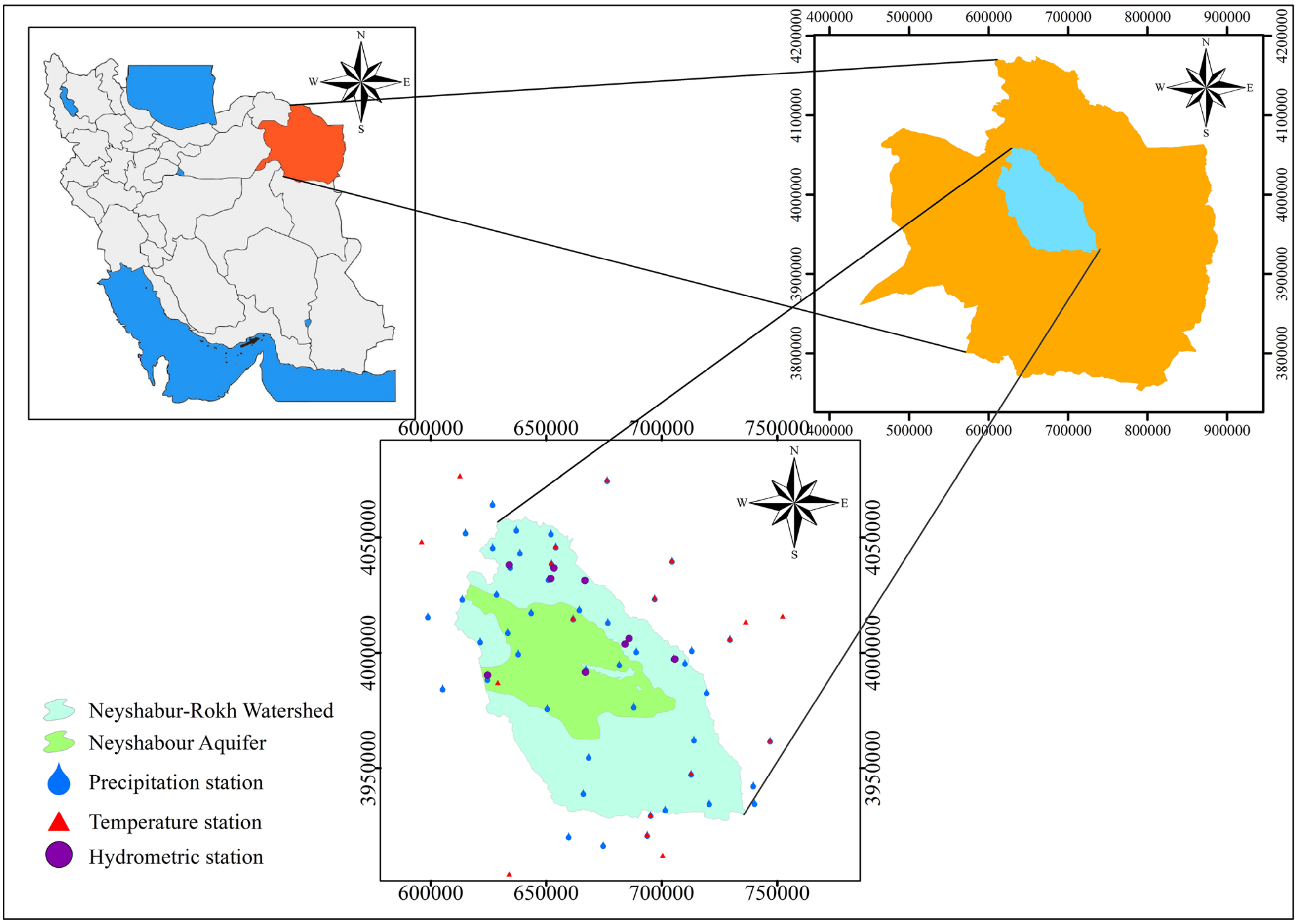

Fig. 1. Location of the Razavi Khorasan province in Iran, the basin in the province and the aquifer in the basin, along with rain gauge, evapotranspiration and hydrometric stations.

Table 1. Statistics of basin water resources

	Well		Qanat		Spring		Total	
Year	Number	Discharge (MCM)	Number	Discharge (MCM)	Number	Discharge (MCM)	Number	Total discharge (MCM)
1968	306	176	438	128			744	304
1981	729	513					729	513
1986	1080	589	568	144	66	41	1648	774
1993	1580	704	628	153	103	28	2208	885
1999	1807	668	619	106	103	15	2529	789
2002	2569	993	894	113	919	61	4382	1167
2008	4057	674	924	67	1107	21	6088	762
2017	3761	514	893	84	988	30	5642	628

considered to be a part of the southern edge of the Binalood geological structure and the northeastern limit of the triangular zone of central Iran in terms of geological divisions (Izady 2014). The Neyshabur watershed is among the agriculturally prone areas in the Razavi Khorasan province, which faced a severe drop in the groundwater level due to excessive exploitation of groundwater resources in the agricultural sector; hence, the Ministry of Energy has designated the area as a critically restricted zone since 1987. Figure 1 shows the boundaries of the Razavi Khorasan province, basin and aquifer, as well as the rain gauge, evapotranspiration and hydrometric stations used in the study.

As can be seen in Table 1, the number of wells has shown a consistent upward trend from 1968 to 2008, with the number increasing in that time by a factor close to 13. The implementation of the groundwater restoration and balancing plan in the basin has halted the rising trend in the number of wells and total discharge, and has partially controlled the exploitation of the aquifer. Figure 2 illustrates the distribution of wells and their increase from 1999 to 2017.

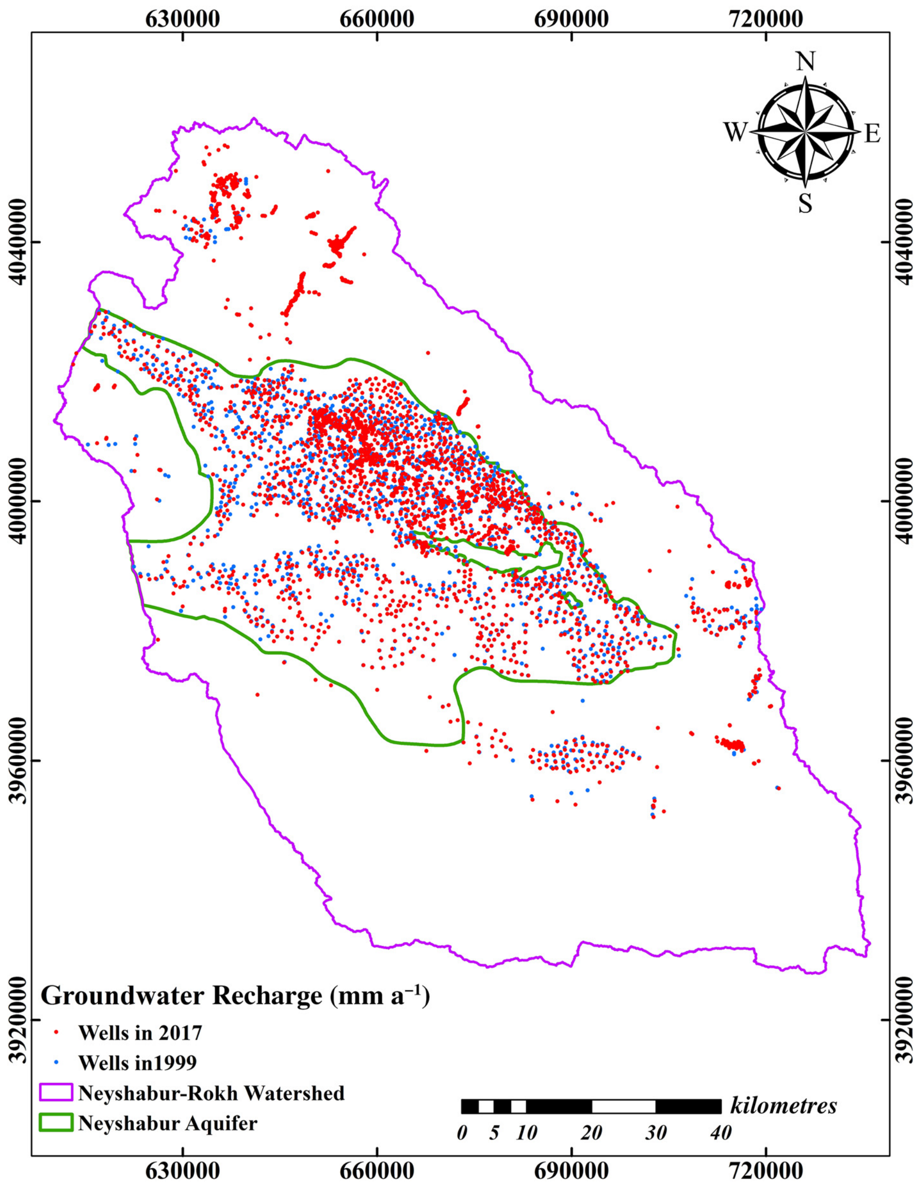

Fig. 2. Distribution of wells in the study area in 1999 and 2017.

Overviewing the WetSpass-M and MODFLOW models

WetSpass-M is regarded as a spatially quasi-steady distributed water balance model that separates precipitation into interception, surface runoff, evapotranspiration and recharge for each cell. In order to consider the heterogeneity of land use in each cell, four subcells including vegetated cover, bare soil, open water and impervious surface are defined for each land-use class (Abdollahi *et al.* 2017). The water balance of a unique raster is achieved by summing the independent water balances of the vegetated cover, bare soil, open water and impervious surface of a raster cell, while the water balance of the studied area is acquired by summing the water balance calculated for each raster cell (Abdollahi *et al.* 2012). Precipitation is considered the starting point for calculating the water balance in a raster cell, and the rest of the processes including interception, runoff, evapotranspiration and recharge are followed regularly. Batelaan and De Smedt (2001) used the WetSpass model for the first time in the Department of Hydrology and Hydraulic Engineering of the University of Brussels to predict hydrological processes in seasonal and annual time steps. The Hydrology and Hydraulic Programming Library (H2PL) then provided the possibility of simulating water balance components including interception, surface runoff, evapotranspiration and recharge on a monthly scale by presenting a new version of the model, namely WetSpass-M, as part of the Python program independent of the Arc view software (Abdollahi *et al.* 2012).

In order to use the finite-difference method in groundwater problems, several practical models have been introduced by the United States Geological Survey (USGS) and these have been made available to all in recent decades. The MODFLOW model has many applications and is widely accepted among hydrogeologists. MODFLOW is a 3D finite-difference model of groundwater flow developed by the USGS (McDonald and Harbaugh 1988) in 1984 utilizing FORTRAN66 (Todd and Mays 2005). Various graphical interfaces were prepared for the MODFLOW code. Groundwater Modelling System (GMS) is considered a comprehensive and user-friendly graphical interface for conducting groundwater simulations. GMS includes several models such as, for example, MODFLOW, MODPATH, FEMWATER and MT3DMS.

The 3D flow of groundwater in a porous medium with constant density is expressed by the following differential equation (Todd and Mays 2005):

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

where K_{xx}, K_{yy} and K_{zz} indicate hydraulic conductivity along the *X*, *Y*, and *Z* axes parallel to the main axes of hydraulic conductivity (LT^{-1}). In addition, h, w, S_s and t represent the hydraulic head (L), the flow flux per unit volume which indicates recharge or discharge (T^{-1}), the special storage of the porous medium (L^{-1}), and time (T), respectively. Equation (1) describes the flow of groundwater under the transient state in a non-homogeneous environment provided that the main axes of hydraulic conductivity are aligned with the coordinate axes. The aforementioned equation takes different forms in steady, transient states, unconfined or confined aquifers. Equation (1) can rarely be solved analytically, except in simple cases. Thus,

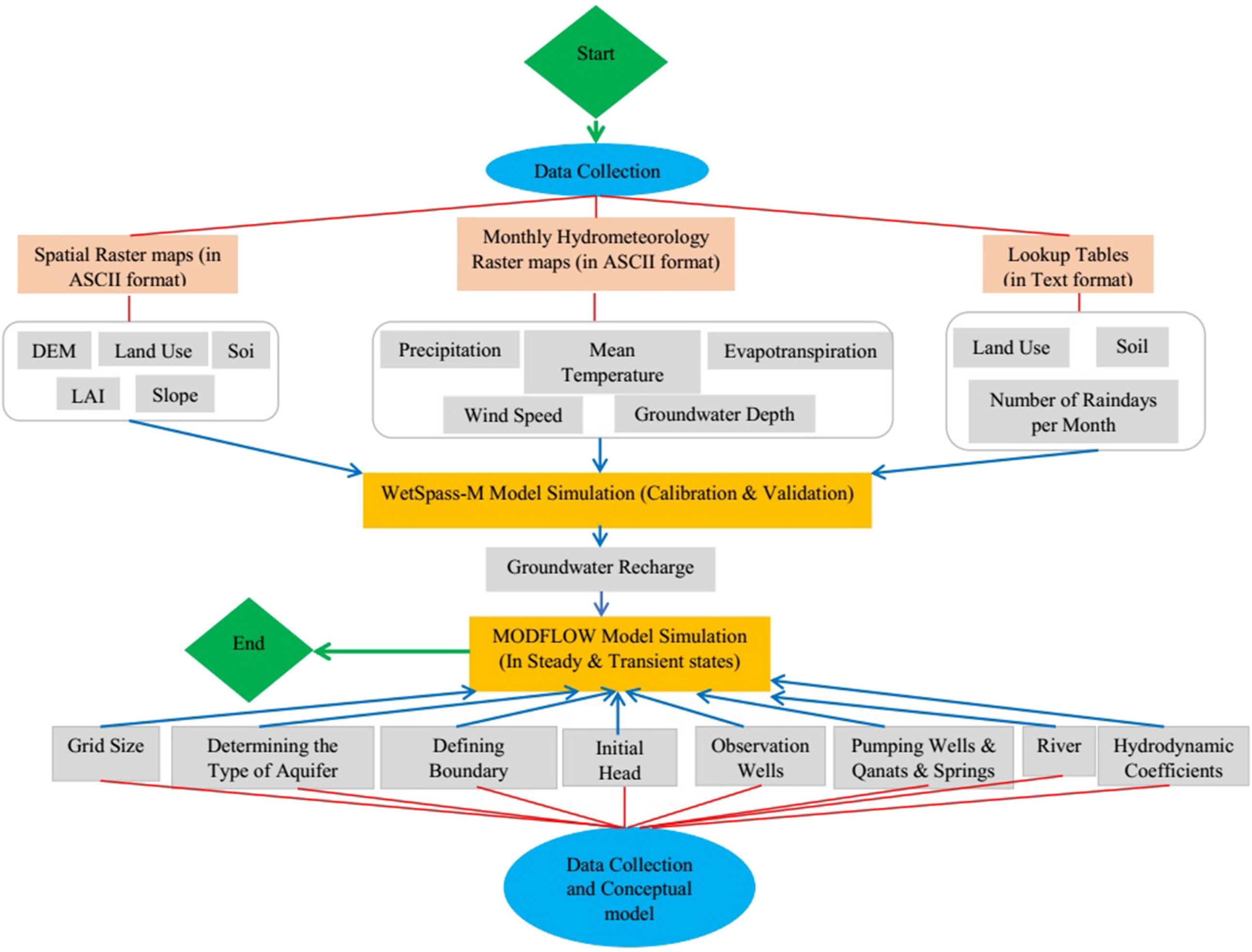

Fig. 3. Flowchart of coupling WetSpass-M and MODFLOW models.

different numerical methods are applied to obtain approximate solutions to solving real problems.

Groundwater recharge

Some researchers have proposed recharge as the main parameter of groundwater (Aslam *et al.* 2022). Achieving accurate information with regard to recharge values is an important step to preparing the appropriate groundwater model (Dowlatabadi and Zomorodian 2016). Groundwater recharge exhibits a stochastic behaviour (Sen 2008) that is influenced by a large number of factors such as weather conditions, land use, soil, and vegetated cover temporally and spatially (Kim *et al.* 2008). Based on the literature review, modellers consider a uniform amount of precipitation for recharge because the above-mentioned factors cannot be applied in groundwater models.

The WetSpass model was developed to simulate long-term average spatial patterns of groundwater recharge (Batelaan and De Smedt 2007). The WetSpass-M model can simulate the interception of vegetated cover, surface runoff, evapotranspiration, soil-water balance and recharge on a monthly scale. The monthly recharge is calculated as the last component of the water balance using the following equation (Abdollahi *et al.* 2012):

$$R_V = P - S_V - ET_V - I \tag{2}$$

where P, I, S_V, ET_V and R_V represent amount of precipitation, interception, surface runoff, evapotranspiration and groundwater recharge (mm/month), respectively. Therefore, the spatial-distributed recharge is estimated based on vegetated cover, soil type, slope, depth of groundwater, and climate variables such as precipitation, evapotranspiration, temperature and wind speed (Abdollahi *et al.* 2012). According to a few studies on the spatio-temporal estimation of groundwater recharge utilizing a distributed hydrological model and its evaluation for the groundwater balance in dry regions with an area of more than 100 km^2 (Hashemi *et al.* 2015) and the successful results of the WetSpass-M model in estimating recharge, the spatio-temporal distribution of the recharge is estimated by WetSpass-M and then used in the MODFLOW model in this study. The cell size considered in both models is 300 × 300 m to increase the accuracy of the input of the distributed recharge values extracted from the WetSpass-M model to input into MODFLOW. The flowchart for the coupling of the WetSpass-M and MODFLOW models is illustrated in Figure 3.

Preparing models input data

WetSpass-M

The WetSpass-M model requires digital elevation method (DEM) maps, slope, land use, soil texture and monthly distribution maps of groundwater depth, the leaf area index (LAI), and climatic data including monthly precipitation, pan evaporation, wind speed and mean temperature during the studied period to simulate the hydrological components of the basin. The DEM map of the SRTM satellite was prepared by the USGS with a resolution of 30 m, and the slope map of the basin was produced using a DEM map in the ArcGIS software. Based on the land use and soil texture maps taken from the Regional Water Company of Khorasan Razavi province, the studied area has 14 land use and six soil texture classes. Poor rangeland and a loam texture are regarded as the dominant land use and soil texture in the area, respectively. The information in the lookup tables of the model was revised based on land use and soil in Iran, and a code was assigned to each class of land use and soil in the region. Daily climate data including precipitation, mean temperature, pan evaporation, wind speed of synoptic stations, climatology, rain gauge and evapotranspiration during 1991–2017 were received from the Iran Meteorological Organization (IRIMO) and the Ministry of Energy. Finally, a number of stations (48, 19, 17 and one) were selected to produce monthly distribution maps of precipitation, mean temperature, evaporation and wind speed, respectively, in the study period after reviewing the received data. The monthly information for the groundwater-level measurement in all of the observation wells of the basin during the studied period was obtained from the Regional

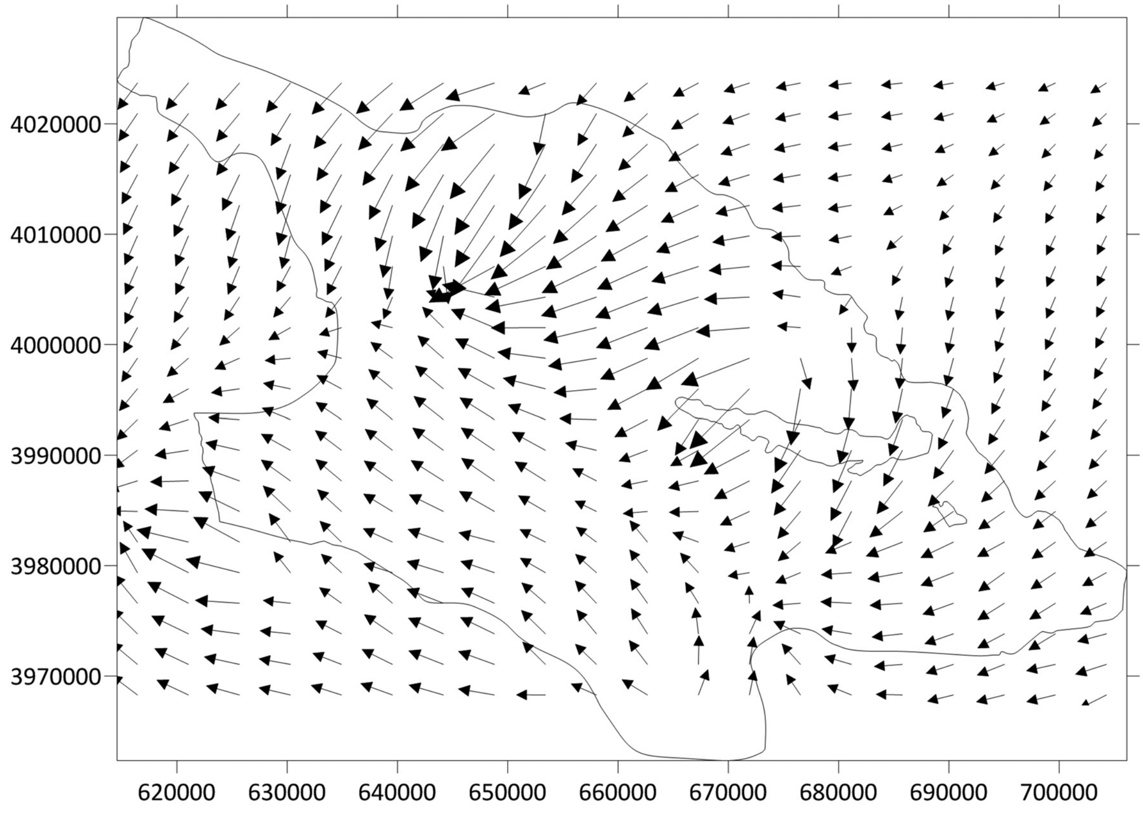

Fig. 4. The groundwater flow direction in the steady state.

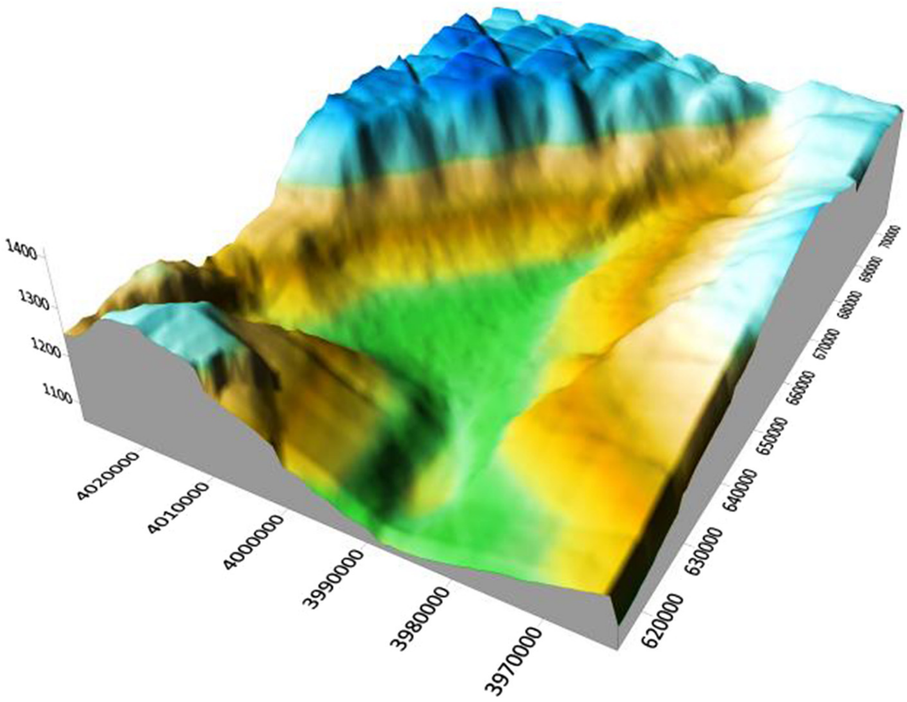

Fig. 5. The 3D topographical map of the Neyshabur aquifer.

Water Company of Khorasan Razavi province, resulting in 29 wells being selected to produce monthly distribution maps of the groundwater level. The monthly LAI map for the studied period was obtained from MODIS (Moderate Resolution Imaging Spectroradiometer). All of the model inputs, except for the number of rainy days, were prepared monthly with a cell size of 300 × 300 m, and 420 columns and 440 rows in a raster map with ASCII format, and introduced into the model. Finally, the model was prepared to begin the hydrological simulation of the basin on a monthly scale by producing and introducing 1948 maps during 1991–2017.

The model outputs included values of direct runoff, groundwater recharge, evapotranspiration and interception, and were presented in each month of the simulation period with their distribution maps in ASCII format. The model was calibrated by comparing the observed and simulated groundwater recharge (base flow) and direct runoff. Therefore, the hydrometric stations in the basin were assessed in terms of the length of the available statistical period, missing data and outlier data test, and five stations were selected to calibrate the model.

MODFLOW

In GMS, there are two methods: a grid and a conceptual model to simulate groundwater. The conceptual model method was used due to its acceptable accuracy in solving real and complex groundwater problems, despite it being more difficult to work with such a method. A conceptual model is considered to be a simplified image of the real world, the preparation of which is regarded as a fundamental step in developing a numerical model in modelling studies. This model is considered as the basis of a mathematical model, which is prepared based on the primary information from field data and hydrogeological

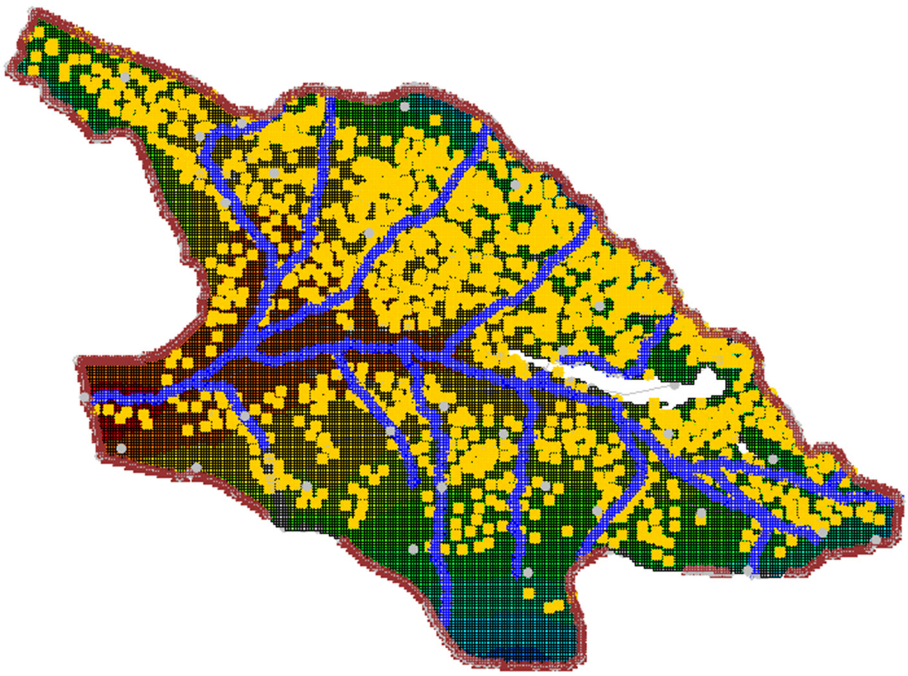

Fig. 6. The conceptual model of the study and finite-difference grid introduced into the MODFLOW model.

Table 2. Allowed range and optimal values related to calibration parameters of WetSpass-M model

Parameter	Optimal value	Allowed range
a (mm)	0.3	0.3–6.5
α (dimensionless)	4	0.3–6.5
LP (dimensionless)	1.22	0.4–5.5
X (dimensionless)	0.635	0–1
β (dimensionless)	0.47	0–1

interpretations. Acquiring correct knowledge with regard to the hydrogeological situation of the region, explaining the problem of groundwater when preparing a numerical model, helping to select an appropriate numerical model and simplifying the problem rationally by utilizing proper hypotheses are among the most critical objectives of preparing a conceptual model. A suitable conceptual model is not necessarily prepared during the first stage of the study. Modelling is regarded as a continuous and dynamic process in which the conceptual model evolves and its constituent hypotheses are re-examined, added, reduced or modified in accordance with the continuation of studies, an increase of knowledge about the system and an increase in the amount of available data (Iran Ministry of Energy 2005). The aquifer boundary in the studied area was determined by reviewing geological maps and the formations therein. The network of observation wells in the Neyshabur aquifer was established and levelled in 1977 to measure changes in the groundwater level (Iran Ministry of Energy 2016). There are now 59 observation wells across the whole of the Neyshabur aquifer, whose groundwater level is measured monthly. Here 28 observation wells that were considered active, and which benefitted from information from 1991 to 2017, were selected and their water level data were prepared during the study period. In addition, October 1999 was regarded as the most stable time after fluctuations in the groundwater level were analysing for the studied time period. Groundwater in the aquifer flows from the north, NE, east and SE to the west and SW, and follows the topography and the network of streams. The boundaries related to the model in all parts, except for small areas in the south of the aquifer, were defined as General Head Boundary by preparing and checking a map for the flow direction of the aquifer in the selected steady time (Fig. 4). The DEM of the SRTM data with a resolution of 30 m received from the USGS was applied to the topography of the aquifer. It is worth noting that the height of the selected observation wells with the DEM map was controlled and corrected when necessary. Figure 5 illustrates the 3D map related to the topography of the aquifer. The bedrock map was prepared using geophysical operation soundings, drilling logs of exploration wells, and its integration with geological and hydrogeological information.

In the steady state, there were generally 1270 water sources, including 1224 wells and 46 qanats in the investigated aquifer. Discharge values of these resources of 25 and 75% were introduced into the model as return water for agricultural and non-agricultural uses, respectively (Iran Ministry of Energy 2010). Owing to the large depth of the water table, evaporation from the groundwater was not performed or considered in the model during the studied period. The river package was utilized to introduce rivers and intermittent streams of the aquifer into the model. The initial values of hydrodynamic coefficients such as the hydraulic conductivity coefficient and specific yield were estimated by the pumping tests performed in the region and then determined during the modelling process and calibrated in the steady and transient states. Information indicated in the GMS 10.5.8 software was recalled and the conceptual model was created. The Neyshabur aquifer as a one-layer unconfined aquifer was divided into a grid containing 247 rows and 336 columns (32 230 active and 50 762 inactive cells) with a size of 300 × 300 m and introduced into the model. Finally, the created finite-difference grid and conceptual model were

Table 3. The values of statistical indicators for evaluating the performance of the model in simulating the monthly total runoff

Name of hydrometric station	Time period	NS	R^2	MB	RMSE
Eriyeh Chaharbagh	1991–2010	0.55	0.59	0.15	0.55
Dizbad Olya	1992–2001	0.5	0.6	0.036	0.14
Zarandeh Andarab	1991–1996	0.5	0.59	0.5	0.48
Eyshabad	1993–2004	0.54	0.63	−0.09	0.9
Kharv Majmo	1992–2003	0.51	0.63	0.45	0.5

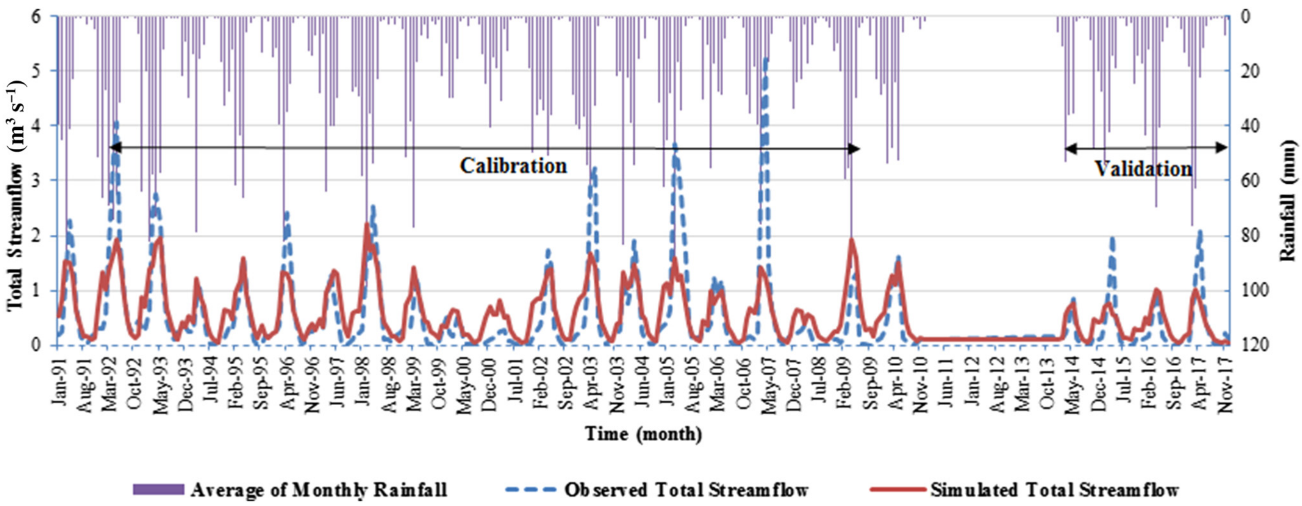

Fig. 7. Comparison of the simulated and observed total runoff at the Eriyeh Chaharbagh station during the calibration (1991–2010) and the validation period (2014–17), along with the average monthly precipitation of the basin.

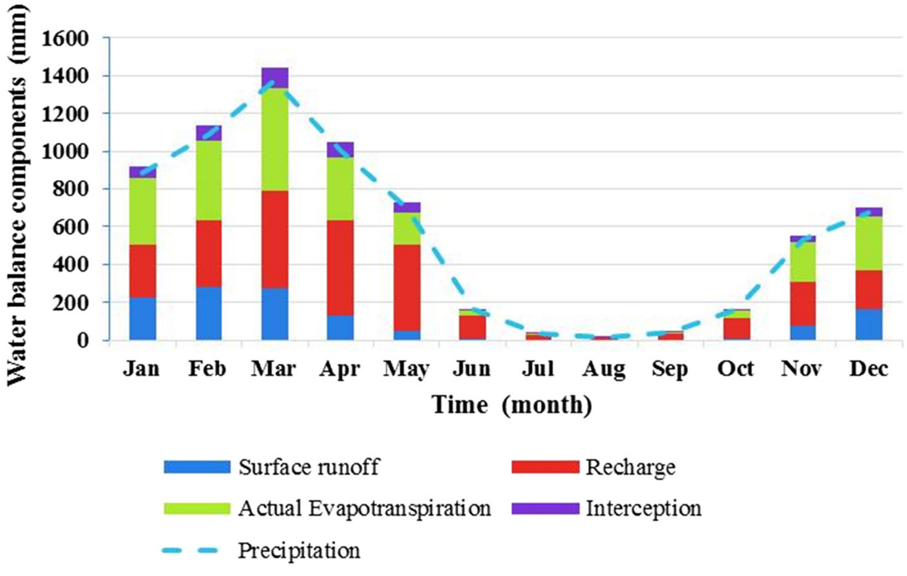

Fig. 8. Monthly distribution of the water balance components in the basin from the total monthly precipitation of the region during 1991–2017.

converted into the MODFLOW-2005 model to begin the simulation (Fig. 6).

Results and discussion

In this study the WetSpass-M and MODFLOW models were coupled to simulate the groundwater flow in the Neyshabur aquifer, which is facing a severe water deficit due to overexploitation and climate change. The models were calibrated and validated using observed data from five hydrometric stations and 28 observation wells. We found that the average annual groundwater recharge was 105.25 mm a^{-1}, which is less than the average annual groundwater withdrawal of 526.5 mm a^{-1}. Results of the models showed good agreement with the observed data, with high values of Nash–Sutcliffe efficiency and coefficient of determination, and low values of error variance, RMSE, ME and MAE. The MODFLOW model sensitivity analysis revealed that the hydraulic conductivity was the most sensitive parameter, followed by the recharge and specific yield. Our study provides a reliable tool for groundwater management and planning in the Neyshabur Basin.

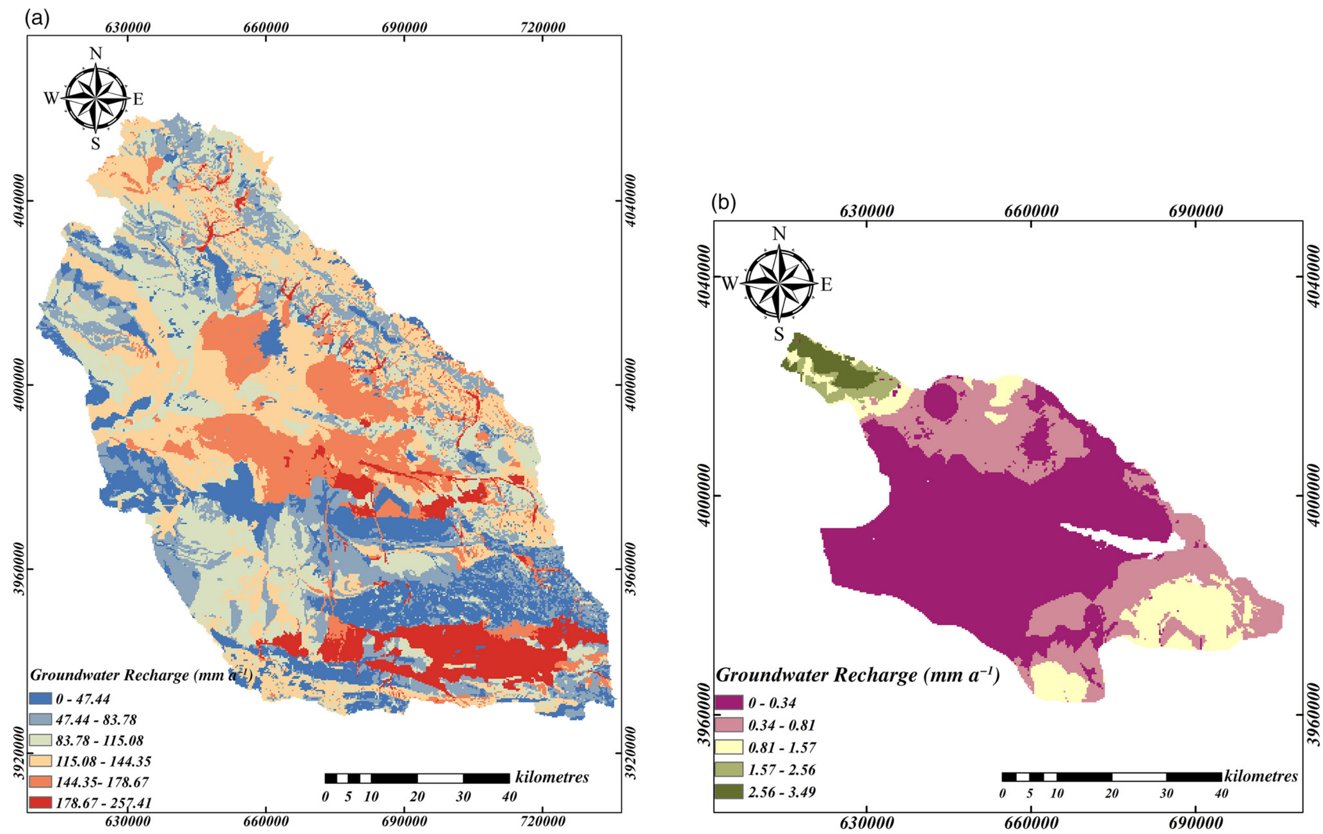

Fig. 9. Spatial distribution map of recharge simulated by WetSpass-M. (**a**) Average annual recharge of the basin during 1991–2017. (**b**) Aquifer recharge in the steady state.

WetSpass-M model calibration and validation

The inputs for the WetSpass-M model for 1991–2017 were prepared, and the model ran on a monthly scale. In order to separate the base flow from the observed discharge, different methods of hydrograph analysis including the local minimum, one parameter digital filter, recursive digital filter, Base Flow Index (BFI) and PART model were evaluated, and the most appropriate method was selected in each station. We calibrated the model manually using a trial and error method by changing the parameters such as interception parameter (a), evapotranspiration coefficient (α), surface runoff (LP), runoff delay factor (x) and base flow (β), and by considering coefficients of Nash–Sutcliffe (NS), coefficient of determination (R^2), the model bias for water balance (MB) and RMSE as objective functions and model performance evaluation criteria in selected hydrometric stations. Table 2 shows the optimal values for the calibration parameters with their allowed ranges.

WetSpass-M model results and discussion

Table 3 represents the values for the evaluation criteria of the model accuracy in simulating the monthly total runoff of the selected hydrometric stations. The Eriyeh Chaharbagh hydrometric station was selected as an appropriate representative of the basin to evaluate the model validation due to its ability to cover the largest sub-basin in the studied area. Evaluation criteria such as NS, R^2, MB and RMSE during the validation period (2014–2017) obtained values of 0.64, 0.5, 0.17 and 0.35 $m^3 s^{-1}$, respectively. Moriasi *et al.* (2007) indicated that the values related to NS should be greater than 0.5 in hydrological studies, as well as pollutant transfer processes on a monthly scale in order to consider the results of the model as acceptable. The same criterion is usually also utilized for the coefficient of determination. According to Table 3, the values of NS and R^2 for all of the stations are greater than 0.5, indicating a satisfactory performance of the model in the simulation. Appropriate values of RMSE and MB as the criteria of model error in simulation for all the hydrometric stations indicate high efficiency, low error and acceptable accuracy of the model during the simulation. The appropriate values of the statistical indices during the calibration of the selected hydrometric stations, as well as their values during the validation of the Eriyeh Chaharbagh station, indicate the high accuracy of the optimized model during calibration and validation.

Figure 7 compares the hydrograph of simulated runoff during the calibration period (1991–2010) and validation (2014–17) with the observed runoff at the Eriyeh Chaharbagh station, along with the average precipitation for the entire basin. The model operated successfully in simulating the process of changes in runoff values, time of occurrence, and peak and minimum discharge values, which play a key role in basin management to confront future floods and droughts in the basin, during the calibration and validation period, so that these changes follow the precipitation pattern of the basin. However, there is a significant difference between the observed and simulated streamflows in April 2007, which is likely be be due to the severe flood that occurred during this time step. Based on the results, the average annual surface runoff, actual evapotranspiration, interception and groundwater recharge during 1991–2017 were 18, 36, 7.6 and 42.6% of the average annual precipitation in the basin, and the simulated water balance error is 4.2%. The results of this research are consistent with the results reported by Bayati (2017), Soleimani Motlagh (2017) and Salem (2022). While Zarei (2016), Ghouili *et al.* (2017), Ashaolu *et al.* (2020), Yenehun *et al.* (2022) and Kisiki *et al.* (2023) introduced actual evapotranspiration, and Zhang *et al.* (2018) presented surface runoff as the component that made the largest contribution to annual precipitation in their studied basin.

Figure 8 demonstrates the portion of the monthly distribution of different water balance components in the basin of the total monthly precipitation of the area during the studied period. As perceived, the lowest amount of monthly recharge occurs during the summer (July–September), probably due to the reduction of vegetated cover and precipitation in the area during this period. The maximum average monthly recharge was observed during March and April with 19.2 and 18.61 mm/month, respectively, which also had high precipitation, while the minimum recharge occurred during August and July with 0.51 and 1.03 mm/month, respectively.

Figure 9a and b shows average annual recharge in the watershed and aquifer. As displayed in Figure 9a, the average annual recharge in the basin due to precipitation varies between 0 and 257.41 mm a^{-1} with an average of 105.25 mm a^{-1}. The spatial distribution map of groundwater recharge extracted from the hydrological model results in October 1999 (steady state) was then prepared as input for the MODFLOW model (Fig. 9b). As observed, the NW areas of the aquifer with their irrigated farming land use have the maximum recharge in a steady state.

MODFLOW model calibration and sensitivity analysis

The conceptual model was converted into a numerical model and the recharge values extracted from the WetSpass-M model were entered in order to calibrate the hydraulic conductivity coefficient of the aquifer. Finally, the MODFLOW model was executed in a steady state. The calibration continued manually (trial and error method) in a logical change and with the input parameters consistent with the characteristics of the region until there was an acceptable match between the observed and calculated water levels

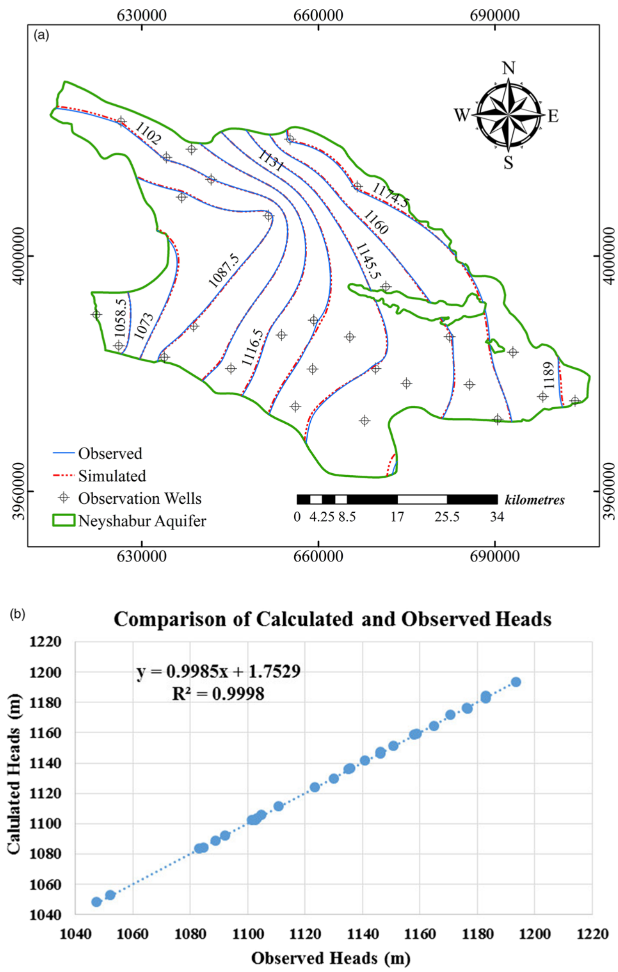

Fig. 10. (**a**) The difference between isopotential lines of the simulated and observed head in a steady state. (**b**) A comparison of the simulated and observed water table.

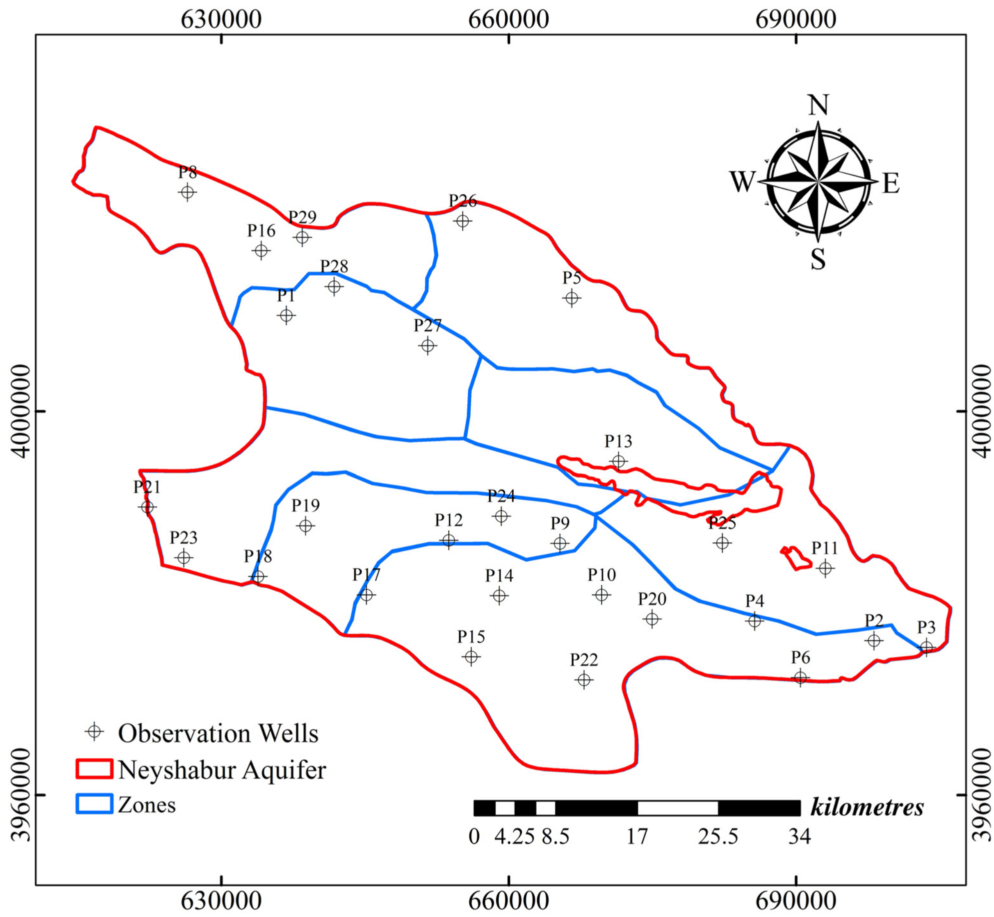

Fig. 11. The zoning considered for the estimation of hydraulic conductivity and specific yield.

in 28 observation wells in the aquifer. It is noteworthy that the recharge values did not change during the calibration of the model.

For calibration of the specific yield coefficient, the model from November 1999–September 2000 was prepared at monthly time steps in a transient state. As the MOFLOW model needs the initial head values to begin the flow simulation (Chiang and Kinzelbach 1998), the simulated water table in a steady state is considered the initial head in the first time step of the transient state. The calculated water table of the previous month is then used as the initial head for the future month.

Most of the parameters used in groundwater modelling such as hydraulic conductivity, specific yield coefficients and recharge have uncertainty. Recognizing such uncertainties and quantifying their change intervals significantly affects the modelling and calibration of these parameters. The calibrated model shows sensitivity to a parameter in which small changes in its values affect the model significantly (Ghodrati and Barzegari 2016).

MODFLOW model results and discussion

The evaluation criteria yielded the following values after model calibration in a steady state: RMSE = 0.55, MAE = 0.48, ME = 0.0018 (in metres), error variance = 0.3 and R^2 = 0.99. Criteria such as error variance, RMSE, ME and MAE indicate the amount of model error in the simulation, and the closer their values are to zero, the more accurate the modelling. Figure 10 shows the difference between isopotential lines of simulated and observed heads, with a comparison chart between the simulated and observed water tables in a steady state after calibration. The values of the evaluation criteria, the greening of the levels in all of the observation wells in MODFLOW model, and good agreement between observed and simulated isopotental lines and groundwater tables (Fig. 10a, b) indicate the appropriate accuracy of the prepared conceptual model, the acceptable performance of the model in simulating a steady state and the accurate estimation of the hydraulic conductivity coefficient of the aquifer.

The zoning considered for the calibration of the hydraulic conductivity coefficient and specific yield is presented in Figure 11. The optimum values of the hydraulic conductivity coefficient and specific yield in different zones, with the observation wells placed in each zone, are indicated in Table 4. The values of the evaluation criteria in the transient state (Table 5) illustrate the appropriate performance of the model prepared for the Neyshabur aquifer in simulating the real conditions of the aquifer. These findings are regarded as more appropriate compared to those reported by Izady *et al.* (2015) in the Neyshabur watershed, in order to apply the simulated recharge using the Soil and Water Assessment Tool (SWAT) in the MODFLOW model, and by Nazarieh *et al.* (2018),

Table 4. Estimated values of hydraulic conductivity and specific yield

Specific yield	Hydraulic conductivity (m/day)	Piezometers in the zone	Zone No
0.1	10.1	p8–p16–p29	1
0.113	7.5	p5–p26	2
0.138	2.5	p1–p27–p28	3
0.185	3	p13	4
0.11	7.5	p21–p23	5
0.26	14.736	p3–p11–p25	6
0.14	18.258	p9–p12–p18–p19–p24	7
0.15	30.55	p2–p4–p6–p10–p14–p15–p17–p20–p22	8

Table 5. Evaluation criteria in transient state after calibration

Stress periods	Error variance	ME	MAE	RMSE
1	0.2554	−0.0295	0.4539	0.5063
2	0.2653	−0.1071	0.4569	0.526
3	0.2538	−0.1793	0.4587	0.5347
4	0.2164	−0.2635	0.4509	0.5346
5	0.2687	−0.3078	0.5039	0.6029
6	0.2754	−0.4428	0.5817	0.6866
7	0.2491	−0.5523	0.6514	0.7445
8	0.2176	−0.4891	0.571	0.6759
9	0.2313	−0.4734	0.5752	0.6748
10	0.2655	−0.4568	0.5755	0.6886
11	0.2494	−0.4863	0.577	0.697
Average	**0.2498**	**−0.3444**	**0.5324**	**0.6247**

indicating the greater accuracy of the WetSpass-M model in estimating recharge.

The results and investigation of hydrographs in all piezometers demonstrate that the model has simulated the variation processes involved at the observed water tables appropriately. For instance, the observed and simulated hydrograph in piezometers 21 and 27 located in the outlet and centre aquifer at the transient state, respectively, are illustrated in Figure 12. In some piezometers, hydrographs of the simulated heads are higher or lower than the observed heads, although both states have occurred in other piezometers. The reasons for these discrepancies include the error caused by not recording the discharge of illegal wells and any carelessness of the operator in recording the water level at the observation wells. The results of the groundwater balance simulated by MODFLOW indicate that the aquifer reservoir faces an annual deficit of 421.3 million cubic metres (MCM), which is equal to an annual drop in the level of the entire aquifer of 97.41 cm. The total results obtained from the simulation of the groundwater flow show a high and suitable ability of the prepared model to simulate the conditions in the Neyshabur aquifer. Further, achieving appropriate values for the evaluation criteria of the groundwater model in steady and transient states indicates a successful coupling of the WetSpass-M and MODFLOW models through the recharge parameter. Aslam *et al.* (2022) and Salem (2022) also reported a desirable performance for the coupling of the WetSpass-M and MODFLOW models in the Chaj Doab area of Pakistan and Drava Basin of Hungary, respectively.

In the sensitivity evaluation, the sensitivity of the model was evaluated by decreasing and increasing the hydraulic conductivity, specific yield and recharge at the levels of 10, 20 and 30% and in a transient state (Fig. 13). Based on the results, the model displays greatest and lowest sensitivity to the hydraulic conductivity coefficient and specific yield, respectively. It is worth noting that the model did not converge while applying a 10% reduction in hydraulic conductivity and a 30% increase in recharge.

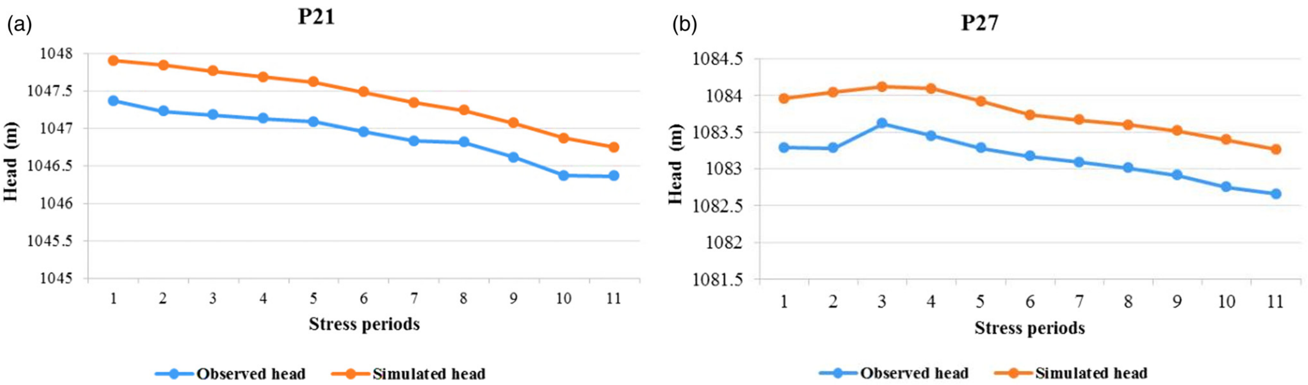

Fig. 12. Hydrographs of observed and simulated heads in (**a**) piezometer 21 and (**b**) piezometer 27 in the transient state.

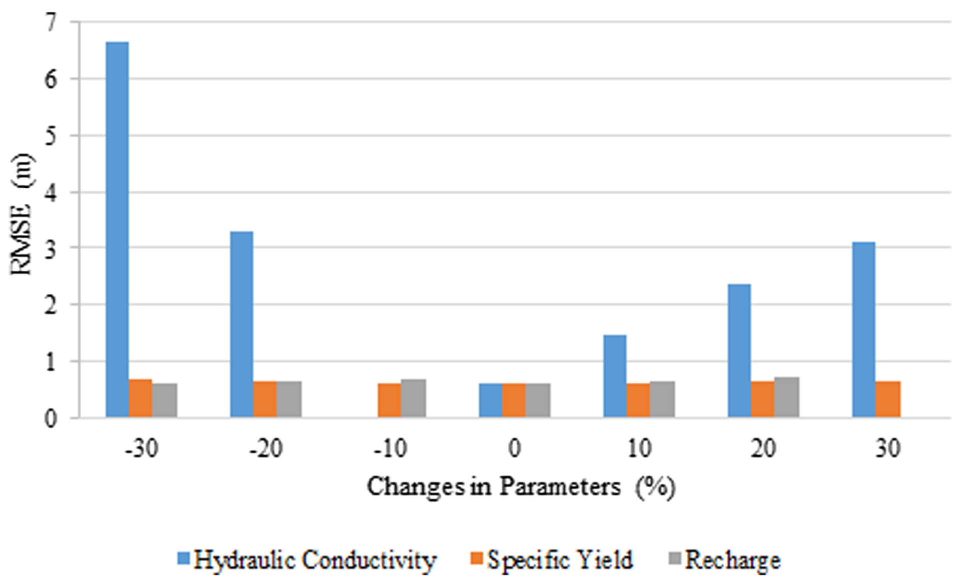

Fig. 13. Model sensitivity analysis of changes in hydraulic conductivity, specific yield and recharge in aquifer.

Conclusion

The high quality, along with the relatively stable state, of groundwater compared to surface water has increased the use of such resources for various objectives, not only in arid and semi-arid countries such as Iran but also in humid climates over the past 50 years. Maintaining these strategic and vital resources requires efficient and effective management. However, sustainable groundwater management needs sufficient and appropriate information about recharge. This study aimed to utilize a combination of a distributed hydrological model and a groundwater flow model in order to estimate the spatio-temporal distribution of recharge and to simulate groundwater flow in the Neyshabur watershed, which is a key basin for providing food security in Razavi Khorasan province. To this aim, we simulated the water balance of the basin during 1991–2017 and the monthly water balance using the WetSpass-M model. The recharge of the aquifer was then extracted from the outputs of the calibrated and validated WetSpass-M model and imported into the MODFLOW model. By calibrating the groundwater model in the steady and transient states, the groundwater balance of the aquifer was simulated and evaluated, and the hydrodynamic coefficient was determined. The simulated water balance of the WetSpass-M model indicates that recharge, actual evapotranspiration, surface runoff and interception form 42.6, 36, 18 and 7.6% of the average annual precipitation in the basin, respectively. The average recharge due to precipitation in the basin is 105.25 mm a^{-1} (303.48 MCM) and the lowest amount of recharge occurs during the summer (July–September). The maximum average monthly recharge is observed during March and April with a value of 19.2 and 18.61 mm a^{-1}, respectively. The groundwater levels, both observed and simulated, were compared in observation wells and in steady and transient states in order to evaluate the coupling of the WetSpass-M and MODFLOW models through the recharge parameter. The appropriate matching of simulated and observed water levels and the suitable values of the evaluation criteria indicate the successful coupling of these models. The groundwater balance simulated by the MODFLOW model illustrates that the aquifer faces a reservoir deficit of 421.3 MCM and a 97.41 cm drop in the groundwater level per year. Of all the parameters, the groundwater model for the basin demonstrated most sensitivity to the hydraulic conductivity coefficient. Due to the major role of recharge in the water balance of the Neyshabur Basin, the results of this study provide a proper understanding of the spatio-temporal distribution of recharge that will assist water resources managers and planners in Iran prevent the continuation of the reservoir deficit by defining appropriate management scenarios and decisions. The maintenance of the reservoir deficit process will lead to a reduction in the quality of groundwater and a threat to agriculture in the basin.

The research encountered several limitations, including an inadequate distribution of stations, observation wells, and the collection and restoration of data. In addition, there was a lack of access to snow melt and irrigation data, as well as to comprehensive bedrock studies. These limitations highlight the need for improved infrastructure and data collection methods to conduct more thorough and precise research in the future. In light of these limitations, the following recommendations are proposed:

- improve the network for measuring hydrometeorology data;
- design a monitoring groundwater level network for the identification and establishment of new observation wells or the elimination of inappropriate, but available, observation wells;
- upgrade the WetSpass-M model on a daily basis for the estimation of daily recharge and to improve groundwater management decisions;
- internal couple the WetSpass-M and MODFLOW models, and presenting them as one program using the Phyton programming language; and
- use the finite-element method rather than finite difference in the simulation of groundwater flow to increase the precision of the definition boundaries.

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Data availability All data generated or analysed during this study are included in this published article (and, if present, its supplementary information files).

References

Abdollahi, K., Bashir, I. and Batelaan, O. 2012. *WetSpass Graphical User Interface*. Department of Hydrology and Hydraulic Engineering, Vrije Universiteit Brussels, Brussels.

Abdollahi, K., Bashir, I., Verbeiren, B., Harouna, M.R., Griensven, A.V., Huysmans, M. and Batelaan, O. 2017. A distributed monthly water balance model: formulation and application on Black Volta Basin. *Environmental Earth Sciences*, **76**, 198, https://doi.org/10.1007/s12665-017-6512-1

Ashaolu, E.D., Olorunfemi, J.F., Ifabiyi, I.P., Abdollahi, K. and Batelaan, O. 2020. Spatial and temporal recharge estimation of the basement complex in Nigeria, West Africa. *Journal of Hydrology: Regional Studies*, **27**, 100658, https://doi.org/10.1016/j.ejrh.2019.100658

Aslam, M., Arshad, M., Singh, V.P. and Shahid, M.A. 2022. Hydrological modeling of aquifer's recharge and discharge potential by coupling WetSpass and MODFLOW for the Chaj Doab, Pakistan. *Sustainability*, **14** , 4421, https://doi.org/10.3390/su14084421

Batelaan, O. and De Smedt, F. 2001. WetSpass: a flexible, GIS based, distributed recharge methodology for regional groundwater modeling. *IAHS Publications*, **269**, 11–18.

Batelaan, O. and De Smedt, F. 2007. GIS-based recharge estimation by coupling surface-subsurface water balances. *Journal of Hydrology*, **337**, 337–355, https://doi.org/10.1016/j.jhydrol.2007.02.001

Bayati, S. 2017. *An Investigation on Distributed Water Balance using WetSpass-M Model (Case Study: Vanak Basin)*. MS thesis, Shahrekord University, Shahrekord, Iran.

Chiang, W.H. and Kinzelbach, W. 1998. *Processing Modflow: A Simulation Program for Modeling Groundwater Flow and Pollution*. Springer, Berlin.

de Vries, J.J. and Simmers, I. 2002. Groundwater recharge: an overview of processes and challenges. *Hydrogeology Journal*, **10**, 5–17, https://doi.org/10.1007/s10040-001-0171-7

Dowlatabadi, S. and Zomorodian, M.A. 2016. Conjunctive simulation of surface water and groundwater using SWAT and MODFLOW in firoozabad watershed. *KSCE Journal of Civil Engineering*, **20**, 485–496, https://doi.org/10.1007/s12205-015-0354-8.

Gelebo, A.H., Kasiviswanathan, K.S. and Khare, D. 2022. Assessment of the spatial–temporal distribution of groundwater recharge in data-scarce large-scale African river basin. *Environmental Monitoring and Assessment*, **194**, 157, https://doi.org/10.1007/s10661-022-09778-z

Ghodrati, M. and Barzegari, F. 2016. *Mathematical Models of Groundwater Applied Learning of GMS 7.1*. Simayedanesh, Tehran.

Ghouili, N., Horriche, F.J., Zammouri, M., Benabdallah, S. and Farhat, B. 2017. Coupling WetSpass and MODFLOW for groundwater recharge assessment: case study of the Takelsa multilayer aquifer, northeastern Tunisia.

Geosciences Journal, **21**, 791–805, https://doi.org/10.1007/s12303-016-0070-5.

Hashemi, H., Uvo, C.B. and Berndtsson, R. 2015. Coupled modeling approach to assess climate change impacts on groundwater recharge and adaptation in arid areas. *Hydrology and Earth System Sciences*, **19**, 4165–4181, https://doi.org/10.5194/hess-19-4165-2015

Iran Ministry of Energy 2005. *Draft Guide of Groundwater Mathematical Model Preparation*. Publication 337. Iran Ministry of Energy, Tehran.

Iran Ministry of Energy 2010. *Studies on the Interconnected Management of Water Resources in Neyshabur Watershed, Volume 3*. Iran Ministry of Energy, Tehran.

Iran Ministry of Energy 2016. *Report of Water Resource Balance of Neyshabur Watershed, Volume 5*, Attachment No, 38. Iran Ministry of Energy, Tehran.

Izady, A. 2014. *Application and Assessment of a Developed Coupled Groundwater–Surface Water Model in the Neishaboor Watershed, Iran*. PhD thesis, Ferdowsi University of Mashhad, Mashhad, Iran.

Izady, A., Davary, K. *et al.* 2015. Groundwater conceptualization and modeling using distributed SWAT-based recharge for the semi-arid agricultural Neishaboor plain, Iran. *Hydrogeology Journal*, **23**, 47–68, https://doi.org/10.1007/s10040-014-1219-9

Kahsay, G.H., Gebreyohannes, T., Gebremedhin, M.A., Gebrekirstos, A., Birhane, E., Gebrewahid, H. and Welegebriel, L. 2018. Spatial groundwater recharge estimation in Raya basin, Northern Ethiopia: an approach using GIS based water balance model. *Sustainable Water Resources Management*, **5**, 961–975, https://doi.org/10.1007/s40899-018-0272-2

Kim, N.W., Chung, I.M., Won, Y.S. and Arnold, J.G. 2008. Development and application of the integrated SWAT–MODFLOW model. *Journal of Hydrology*, **356**, 1–16, https://doi.org/10.1016/j.jhydrol.2008.02.024

Kisiki, C.P., Ayenew, T. and Mjemah, I.C. 2023. Estimation of groundwater recharge variability using a GIS-based distributed water balance model in Makutupora basin, Tanzania. *Heliyon*, **9**, E15117, https://doi.org/10.1016/j.heliyon.2023.e15117

McDonald, M.G. and Harbaugh, A.W. 1988. A modular three-dimensional finite-difference groundwater flow model. *In*: *Techniques of Water Resources Investigation, Book 6*. United States Geological Survey, Reston, VA, Chapter A1.

Moriasi, D.N., Arnold, J.G., Van Liew, M.W., Bingner, R.L., Harmel, R.D. and Veith, T.L. 2007. Model evaluation guidelines for systematic quantification of accuracy in watershed simulations. *Journal of American Society of Agricultural and Biological Engineers*, **50**, 885–900, https://doi.org/10.13031/2013.23153

Nazarieh, F., Ansari, H., Ziaei, A.N., Izady, A., Davari, K. and Brunner, P. 2018. Spatial and temporal dynamics of deep percolation, lag time and recharge in an irrigated semi-arid region. *Hydrogeology Journal*, **26**, 2507–2520, https://doi.org/10.1007/s10040-018-1789-z

Salem, A. 2022. *A Fully Distributed Integrated Hydrologic Model for Integrated Water Resources Management in a Highly Regulated River Floodplain*. PhD thesis, University of Pécs, Pécs, Hungary.

Salem, A., Dezsö, J. and El-Rawy, M. 2019. Assessment of groundwater recharge, evaporation, and runoff in the Drava Basin in Hungary with the WetSpass Model. *Hydrology*, **6**, 23, https://doi.org/10.3390/hydrology6010023

Sen, Z. 2008. *Wadi Hydrology*. 1st edn. CRC Press, Boca Raton, https://doi.org/10.1201/9781420061550

Shah, T. 2014. *Groundwater Governance and Irrigated Agriculture*. TEC Background Papers, **19**. Global Water Partnership, Technical Committee (TEC), Stockholm.

Shrestha, S., Bach, T.V. and Pandey, V.P. 2016. Climate change impacts on groundwater resources in Mekong Delta under representative concentration pathways (RCPs) scenarios. *Environmental Science & Policy*, **61**, 1–13, https://doi.org/10.1016/j.envsci.2016.03.010

Siebert, S., Burke, J., Faures, J.M., Frenken, K., Hoogeveen, J., Döll, P. and Portmann, F.T. 2010. Groundwater use for irrigation – a global inventory. *Hydrology Earth and System Sciences*, **14**, 1863–1880, https://doi.org/10.5194/hess-14-1863-2010

Soleimani Motlagh, M. 2017. *Evaluation of Groundwater Budget with Emphasis on the Separation of Deficit Caused by Drought and Overexploitation of Aquifer (Case study: Alashtar Plain)*. PhD thesis, University of Kashan, Kashan, Iran.

Sophocleous, M. 2005. Groundwater recharge and sustainability in the High Palin aquifer in Kansas, USA. *Hydrogeology Journal*, **13**, 351–365, https://doi.org/10.1007/s10040-004-0385-6

Tilahun, K. and Merkel, B.J. 2009. Estimation of groundwater recharge using a GIS-based distributed water balance model in Dire Dawa, Ethiopia. *Hydrogeology Journal*, **17**, 443–1457, https://doi.org/10.1007/s10040-009-0455-x

Todd, D.K. and Mays, L.W. 2005. *Groundwater Hydrology*. John Wiley & Sons, Hoboken, NJ.

Yenehun, A., Dessie, M. *et al.* 2022. Spatial and temporal simulation of groundwater recharge and cross-validation with point estimations in volcanic aquifers with variable topography. *Journal of Hydrology: Regional Studies*, **42**, 101142, https://doi.org/10.1016/j.ejrh.2022.101142

Zarei, M. 2016. Estimating groundwater recharge, evapotranspiration and surface runoff using land-use data: a case study in northeast Iran. *Biological Forum*, **8**, 196–202.

Zhang, Y., Liu, S., Cheng, F. and Shen, Z. 2018. WetSpass-based study of the effects of urbanization on the water balance components at regional and quadrat scales in Beijing, China. *Water*, **10**, https://doi.org/10.3390/w10010005