



Research Article

Determination of the travel time and path of pollution in Iranshahr aquifer by particle-tracking model



Amin Mohebbi Tafreshi¹  · Mohammad Nakhaei²  · Mahdi Lashkari³ · Ghazaleh Mohebbi Tafreshi¹ 

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Abstract

Recognitions and predictions of the contamination origin are essential steps in the protective measures to avoid well-water contamination and the first step in managing groundwater resources. In this regard, finite-difference model software (GMS 10.0.6) was used to model the transport path, the origin of contaminants and to determine the wellhead protection area in Iranshahr aquifer. Since contamination transport models require a calibrated groundwater flow model, we first prepared this model. Accordingly, after collecting all geological, meteorological, hydrological and hydrogeological data (based on the maps, geophysical tests and exploratory borehole drilling, rainfall statistics and groundwater level in exploitation wells), a database was constructed in ArcGis10.1 software and a conceptual model was developed by transporting this information to GMS software. Based on the developed model, the aquifer's groundwater level was simulated, calibrated and validated using MODFLOW2000 code in GMS software. The particle transport model in the aquifer was provided to examine and model the transport path and the origin of contaminants through MODPATH module. In the end, the aquifer wells' protection area against contaminants was illustrated. According to the results, contaminant transport path in the wells of central plains is directed from the river to the wells, in forward particle-tracking model; the maximum time taken by particles is 508,952.5 days, the minimum time is 144 days, and the average radius of 50-day wellhead protection area based on the protection against contaminations such as pathogenic bacteria in Iranshahr aquifer was determined to be about 100 m.

Keywords Groundwater flow model · Particle-tracking model · Groundwater modeling system · MODPATH · Wellhead protection area

1 Introduction

Since groundwater is exposed to severe contamination, effective strategies are required to manage and protect these resources to avoid irreversible environmental effects, such as a sharp decline in the quality of these waters and their destruction [25]. Thus, in order to protect and preserve these natural resources, accurate monitoring and evaluation should be performed using mathematical and numerical modeling based on which the managers can

adopt proper strategies for future management decisions [26]. Recognition of the contamination origin and transport path is among the first measures to avoid any groundwater contamination risk, based on which protection areas could be considered, and necessary measures could be taken.

Due to the importance of public water supply wells, especially in a dry region such as Sistan and Baluchestan province of Iran, protection from pollution in these resources is very important. Based on this, the Wellhead

✉ Amin Mohebbi Tafreshi, std_a.mohebbi63@khu.ac.ir; Mohammad Nakhaei, nakhaei@khu.ac.ir; Mahdi Lashkari, lashkari@moe.gov.ir; Ghazaleh Mohebbi Tafreshi, std_gh.mohebbi@khu.ac.ir | ¹Department of Applied Geology, College of Earth Sciences, Kharazmi University, Tehran, Iran. ²Department of Applied Geology, College of Earth Sciences, Kharazmi University, Tehran, Iran. ³Expert of Ministry of Energy, Tehran, Iran.



Protection Area (WHPA) seems like a practical protection strategy. The Wellhead Protection (WHP) means the protection of groundwater surrounding the public water supply wells, known as the Wellhead Protection Area [37, 38]. There are dozens of local and international publications within this field [5, 9, 16, 28, 30], including that of Rajkumar and Xu [35] which aimed to establish an integrated method that defines: first of all, the areas of highest vulnerability in the aquifer, and second, within these areas, the wells that most urgently need protection. To identify these wells, additional criteria were taken into consideration, such as well constructive data, pumped volume, and the region's socioeconomic characteristics (social exclusion index). Once the wells were ranked, many of them were chosen as a pilot study to compare different methods for the delineation of WHPA based on calculated fixed radius and analytical methods. In this way, it is possible to identify which method or methods best adapt to the characteristics of the study area. In another study [10], several methods were compared to determine wellhead protection area in a different period of time in drinking water wells in some parts of Tehran in Iran. Due to the high precision and validity of the numeric model results in determining wellhead protection area, they compared the precision and validity of the other methods of wellhead protection area determination with the numerical model results in MODPATH model [32], and finally, they selected the most consistent method during distinct times for determining qualitative wellhead protection area. Countryman [7] in a research conducted in Santa Rosa County in northwestern Florida, USA, determined the wellhead protection area using MODPATH model. Other researchers studied the origin of contaminants and determined wellhead protection area [1, 2, 6, 8, 11–14, 23, 31, 33, 36, 39–41, 43].

Based on the mentioned cases and considering that there is no tracing test in the study area, mathematical modeling can be used as a suitable alternative method to define the source and path of pollution. In this regard, the aim of this research is to simulate groundwater flow in Iranshahr aquifer to model the contaminant transport path in order to identify the origin of contaminants and determine the wellhead protection area using the Groundwater Modeling System (GMS) software.

2 Materials and methods

2.1 Location

The studied aquifer is located within the city of Iranshahr, Sistan Baluchistan Province, in southeast Iran and is considered a part of Iranshahr Basin (Fig. 1). Iranshahr aquifer with an area of about 409 km² is located 345 km from the

city of Zahedan, capital of Sistan and Baluchistan province at coordinates between Latitude 258280 to 288530 and Longitude 2996540 to 3022950 in 41 N zone based on Universal Transverse Mercator (UTM) system.

2.2 Climate, topography, and drainage

Iranshahr aquifer has an average altitude of 591.1 m above sea level [29]. This area with an annual average rainfall of 112 mm (Fig. 2) and an annual average temperature of 26.9 °C (Fig. 3) [29] falls into dry climate (De Martonne classification) and hot middle equatorial climate (Emberger revision). Its topographic slope is directed from the north, east and south regions to the center of the aquifer. Bampoor River is the main drainage system in Iranshahr aquifer. The river drainage starts from the southeastern Iranshahr, 9 km before Bampoor Dam and continues up to 2 km after Bampoor Dam.

2.3 Geology

The study area is located in the east Hamoon–Jazmuriyan embayment. In this area, geologic units could be seen in the highlands at the margins of the aquifer. The oldest geological formations of the region belong to the Late Cretaceous–Oligocene, including gabbro, diorite to granodiorite, and alkali granite porphyry (Fig. 4). The formations are made of sedimentary rocks such as sandstone and interior and extrusive basic igneous rocks [15]. The maximum spreads of deposits are visible in the northern part in the region, and external volcanic formations are in the eastern and southern regions of the plain. This area is affected by Alpine orogenic movements so that most of these activities can be seen in the northern parts of Iranshahr. There is no sign of quaternary volcanic activities within this area [29].

2.4 Hydrogeology

According to the logs that were recorded by Sistan and Baluchistan Regional Water Authority in 2011 using the geoelectric method by performing about 55 geoelectrical catheterizations in six lines [15], the mentioned aquifer is a single-layer unconfined aquifer. Based on the data of depth to water table contour map, the aquifer's hydraulic gradient is generally directed from the north and east to the west [15]. In the west Bampoor River, the aquifer's groundwater table turns into a relatively narrow 5 km wide valley to the river bed, due to the reduced width of the alluvial bed. In fact, at this point, the reduction in the groundwater reservoir's width and the aquifer's thickness has led to the limited hydraulic connection between groundwater tables in the east and west areas. Thus, the

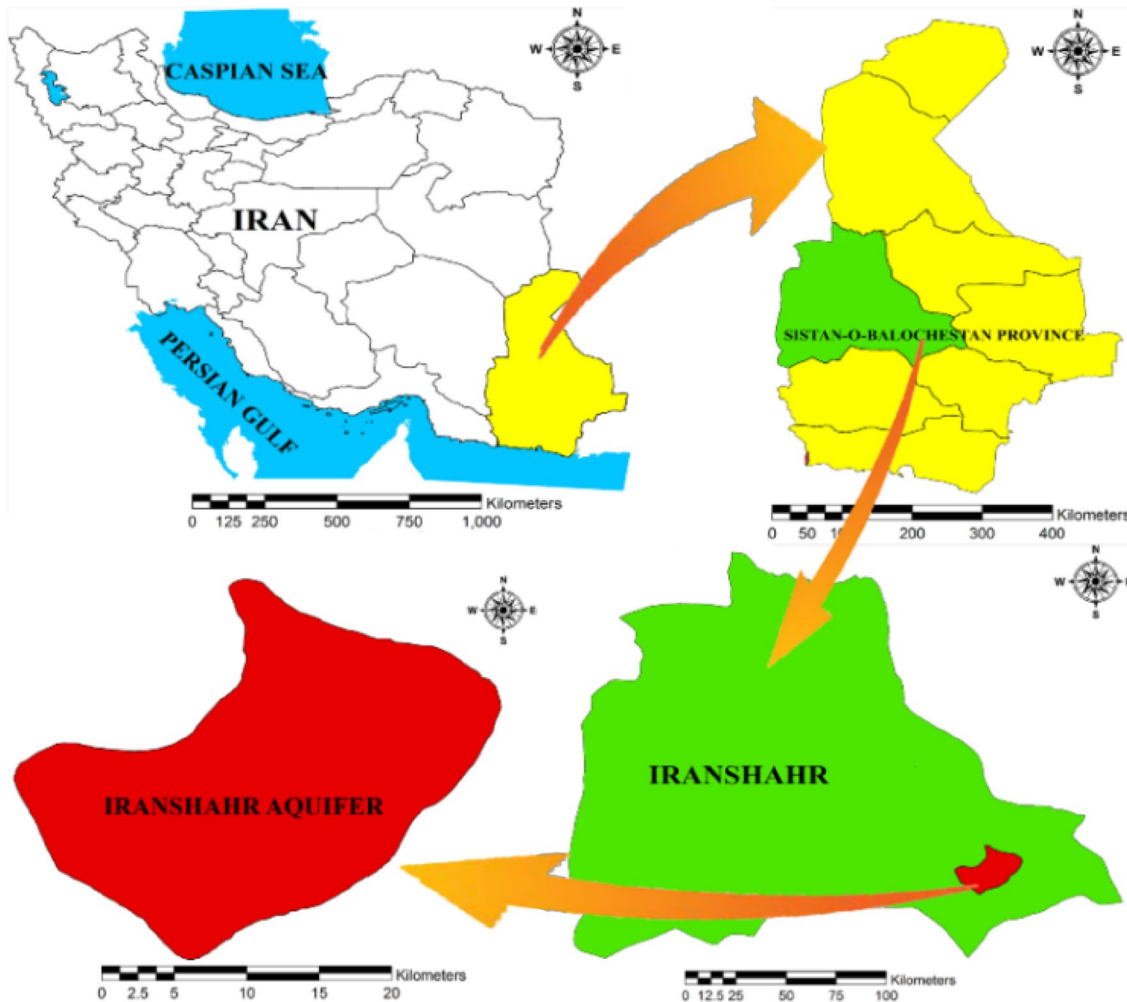


Fig. 1 Location of the study area

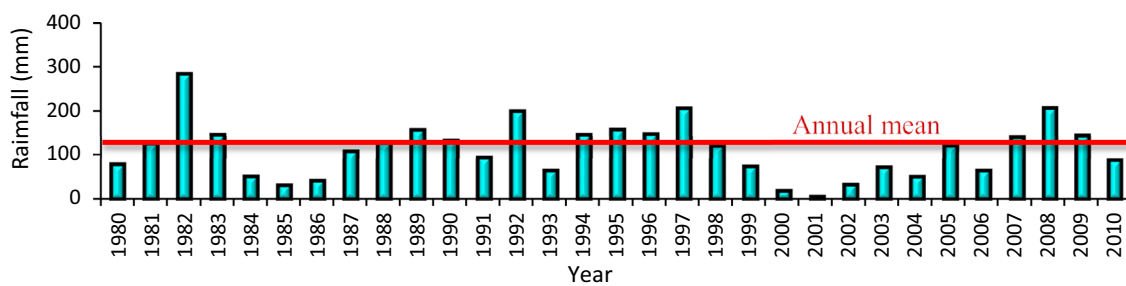


Fig. 2 Variations of annual rainfall (Iranshahr station)

groundwater site is selected as the Iranshahr aquifer limit with regional western plains.

2.5 Sampling and method of analysis

Since contamination transport models require a calibrated groundwater flow model [18, 27], the flow model was first

prepared in the study area. The MODFLOW code [24] was used for groundwater flow modeling. The governing equation in this modeling is Poisson's equation in the 3D state which is as follows [24]:

$$\frac{\partial}{\partial x} h \frac{\partial h}{\partial x} + \frac{\partial}{\partial y} h \frac{\partial h}{\partial y} + \frac{\partial}{\partial z} h \frac{\partial h}{\partial z} = Sy \frac{\partial h}{\partial t} \pm \frac{R}{2K_{x,y}} \tag{1}$$

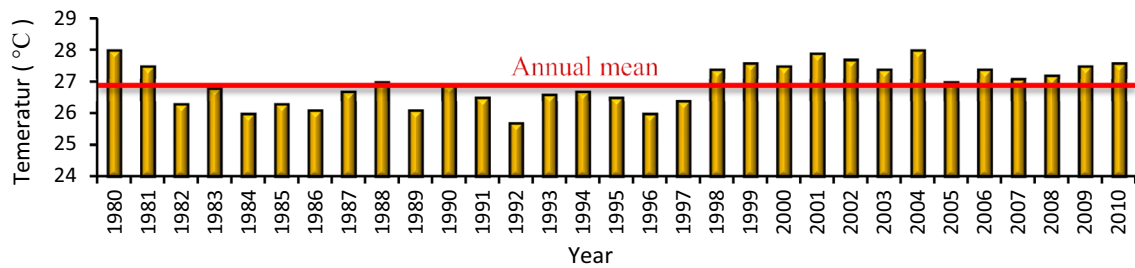


Fig. 3 Variations of annual temperature (Iranshahr station)

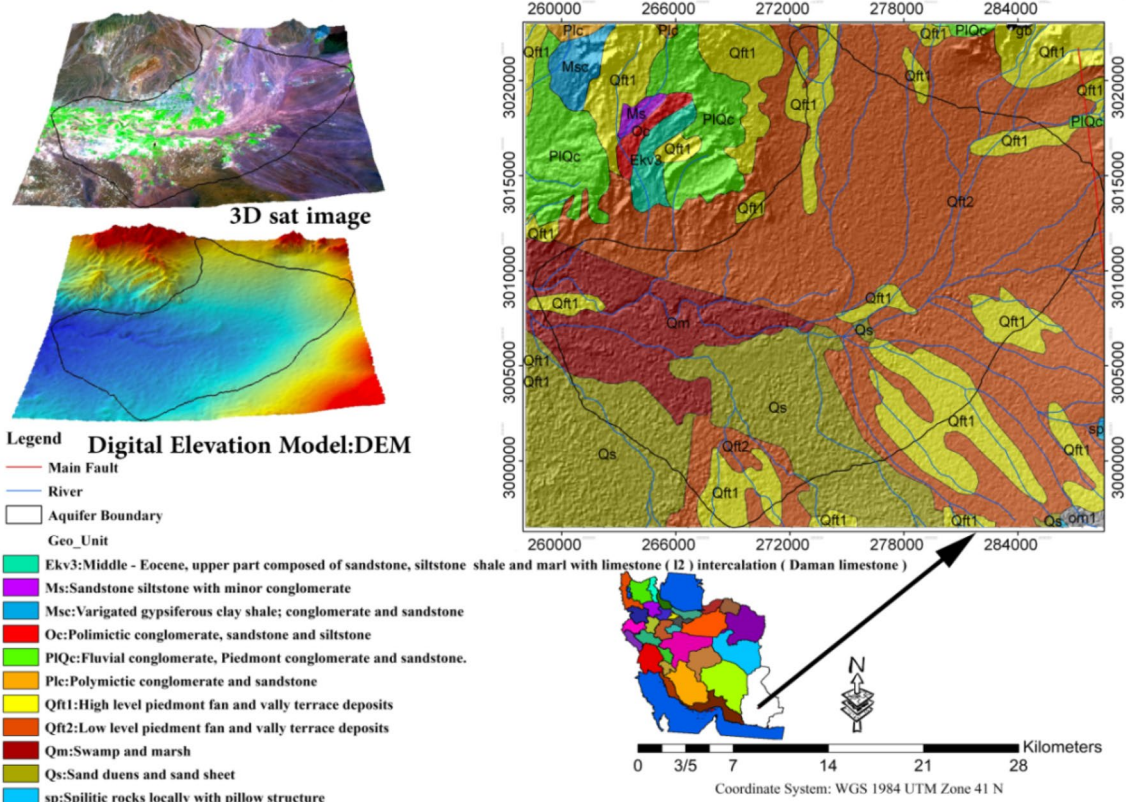


Fig. 4 The geology map of the study area

where $K_{x,y}$ is the component of hydraulic conductivity in x and y directions, $\frac{\partial}{\partial x} h \frac{\partial h}{\partial x}$ is the second-order partial derivative of the hydraulic head toward in the direction of x , $\frac{\partial}{\partial y} h \frac{\partial h}{\partial y}$ is the second-order partial derivative of the hydraulic head toward in the direction of y , $\frac{\partial}{\partial z} h \frac{\partial h}{\partial z}$ is the second-order partial derivative of hydraulic head toward in the direction of z , S_y is specific yield (in the unconfined aquifer), and R is the recharge (+) or the discharge (-) component of the aquifer.

In the following, a database was prepared in ArcGIS v.10.1 software [34] using all available information such as

1:100,000 geological map of the study area [17], monthly hydrological and meteorological statistics in 2004–2014 (taken from the Sistan and Baluchestan Regional Water Authority), Enhanced thematic mapper (ETM) satellite images, Google Earth satellite images, geophysical exploration surveys [29], hydrogeological studies and balance using groundwater levels in observation wells since 2004 to 2014 (taken from the Sistan and Baluchestan Regional Water Authority). Using Aquaveo GMS v.10.0.6 software [3], the information stored within the GIS database was converted into a conceptual model. Then, the obtained model changed into numerical model arrays, and the model

was implemented, calibrated and verified using the Modflow2000 module in GMS software. To show the calibration process, GMS software uses colored rods in observation wells (Figs. 5, 9) that display the rate of calibration error where its center matches the observed values [20].

For modeling the transport path, the origin was determined through backward and forward methods in MODPATH module of GMS software. Meanwhile, the same module was used to determine the wellhead protection area. The equations used in this module that described the particle-tracking algorithm are as follows [32]:

$$\frac{\partial}{\partial x}(nv_x) + \frac{\partial}{\partial y}(nv_y) + \frac{\partial}{\partial z}(nv_z) = W \tag{2}$$

where v_x , v_y , and v_z are the principal components of the average linear groundwater velocity vector, n is porosity,

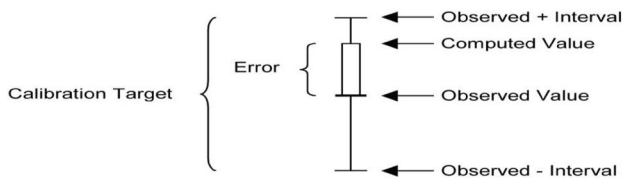


Fig. 5 The calibration symbol in GMS software [20]

and W is the volume rate of water created or consumed by internal sources and sinks per unit volume of the aquifer.

In Fig. 6, different stages of research are shown.

3 Results and discussion

3.1 Flow model

The model of the study area was implemented according to the protocol presented by Wang and Anderson [42]. Given the Iranshahr aquifer status, existing data, study objectives, and geometric shape of the aquifer, a finite-difference network with dimensions of 61 columns and 53 rows was developed after the preparation of the conceptual model. In this study, cell dimensions for both flow and transport models were considered the same and 500 m × 500 m. According to this disaggregation, the network-forming cells are 3230 ones among which—according to the model borders—1614 active cells and 1616 inactive cells were introduced to the model. According to the geophysical studies, drilling logs and topography of upper and lower levels of the aquifer (Fig. 7), the aquifer thickness varies from maximum 240 m in the central regions to a minimum 40 m at the western Strait at the end of the aquifer. In this study, the zoning method was used to

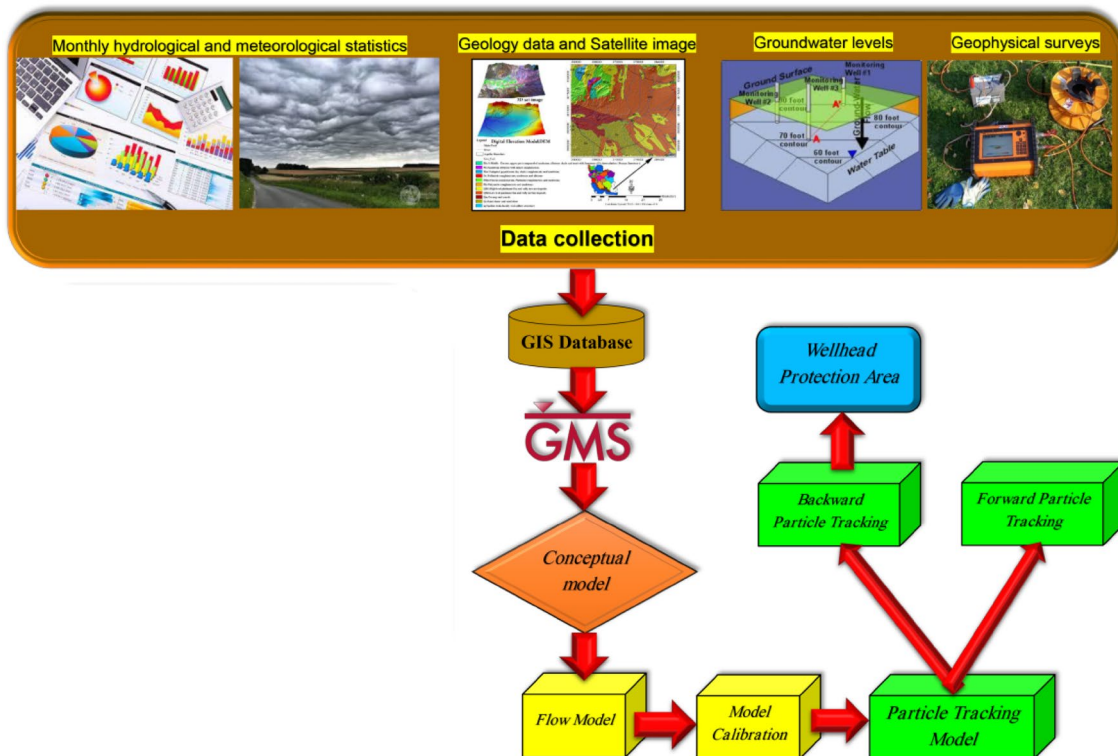


Fig. 6 The flowchart of the methodology

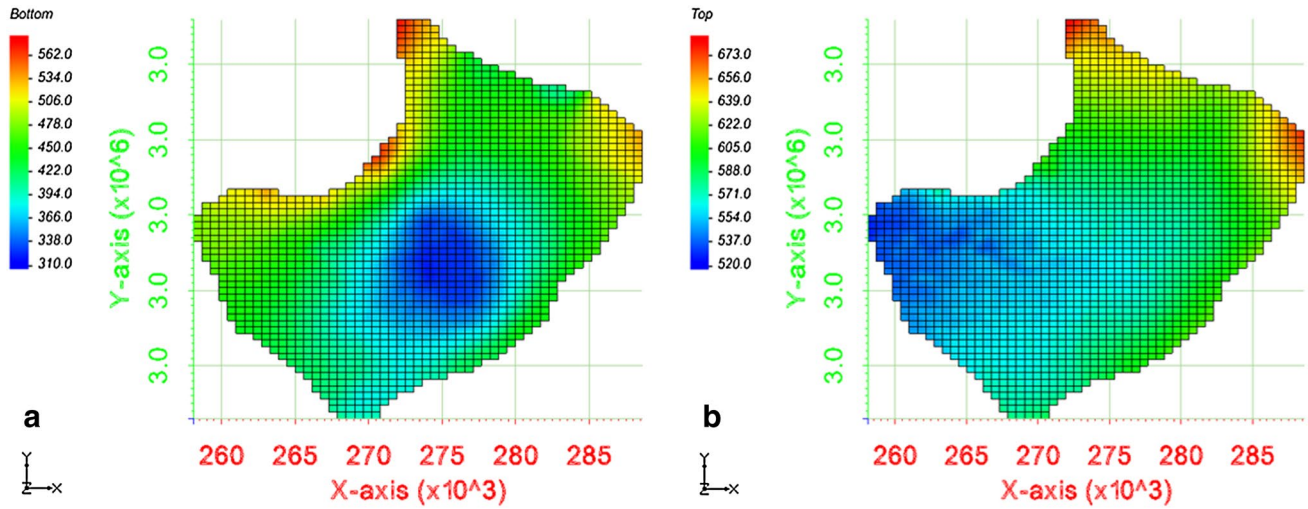


Fig. 7 The bottom (a) and top surface (b) topography of the study area

estimate and optimize the hydraulic conductivity (K) values. In this method, some points within the aquifer area that are similar relatively and lithologically are defined as a zone for which a “ K ” value is determined. Accordingly, five hydraulic conductivity zones were defined based on the data obtained from drilling logs as well as field studies for the model area (Fig. 8). There are 207 exploitation wells within the study area which were introduced as abstraction wells, and their harvest discharge was included in the model.

Meanwhile, Bampoor River—which begins at the confluence of the rivers in the North and East aquifer and exits

from the western end of the aquifer—was introduced to the model in two parts of river (from the north to the center of the aquifer) and drain (from the center to the western end of the aquifer) due to its hydraulic properties. According to rainfall, evapotranspiration and transpiration, agricultural returned water, as well as the aquifer’s permeability, 0.000085 m/d, were introduced into the model as recharge. For steady-state implementation of the model, monthly statistics of the plane’s observation wells related to 2004 were used as the modeling origin and were implemented. For transient-state implementation of the model, a period of 365 days and 12 stress periods were selected

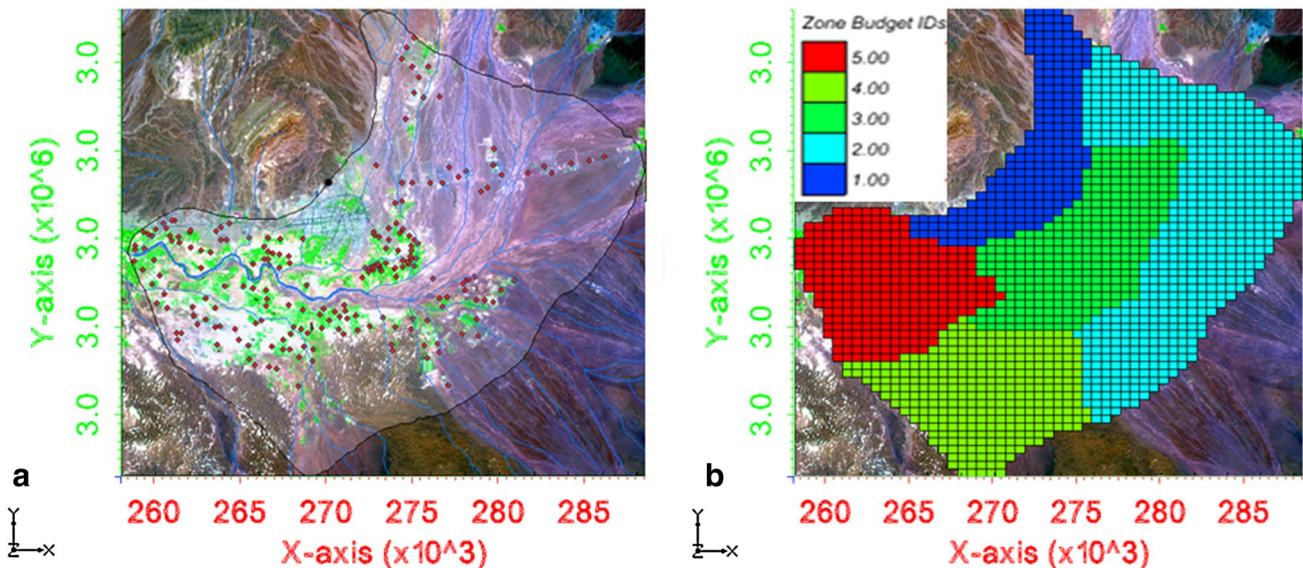


Fig. 8 Location of exploitation wells and Bampoor River (a) and zoning aquifer in terms of hydraulic conductivity (b)

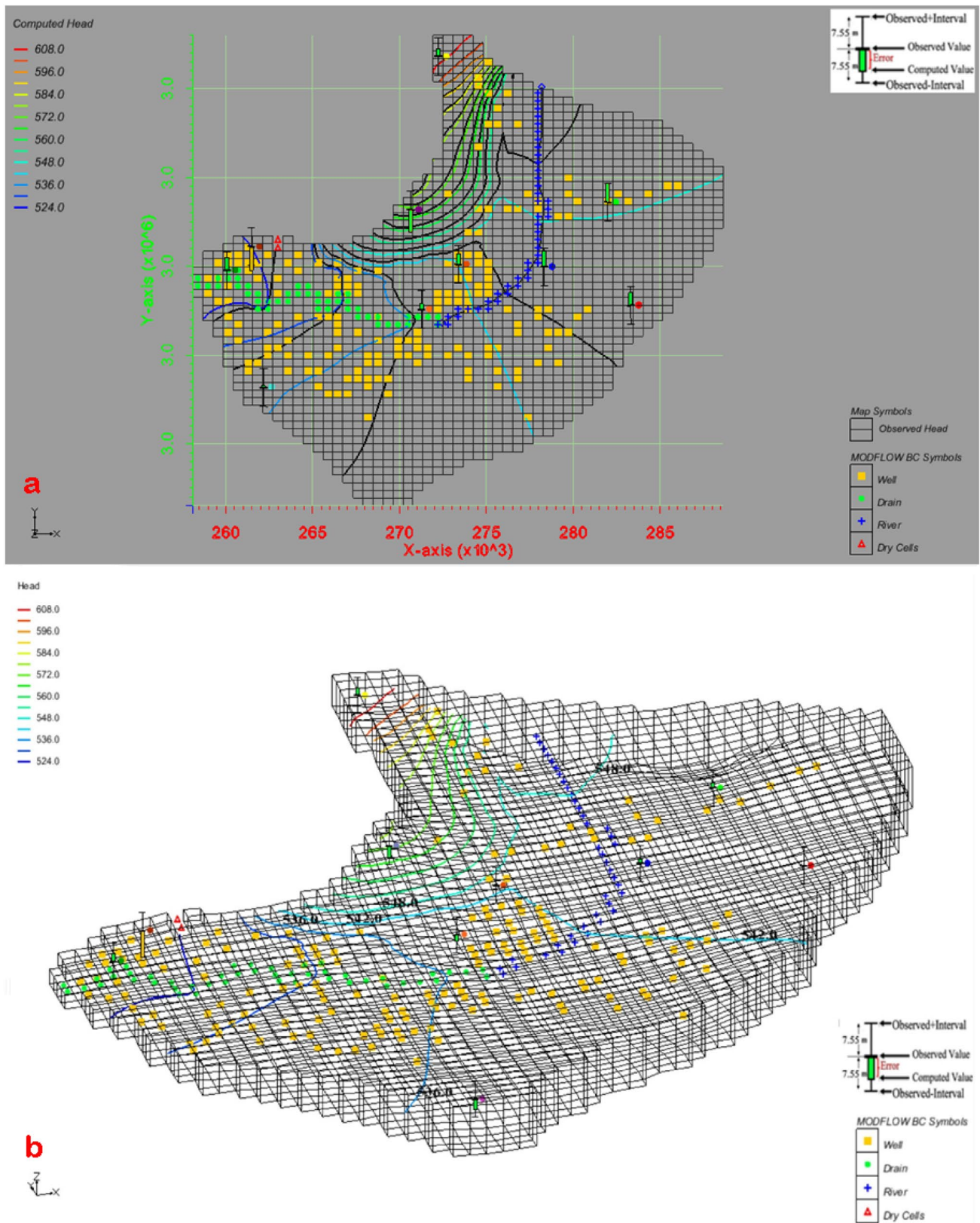


Fig. 9 a Initial observed hydraulic head (black lines) and calculated hydraulic head by the model after calibration (colored lines). According to colored rods in observation wells, the error in most

wells is less than the acceptable error, and calibration is excellent; **b** 3D view of the calculated hydraulic head by the model after calibration

Table 1 Optimized value of the parameters *K* and *Sy* after calibration

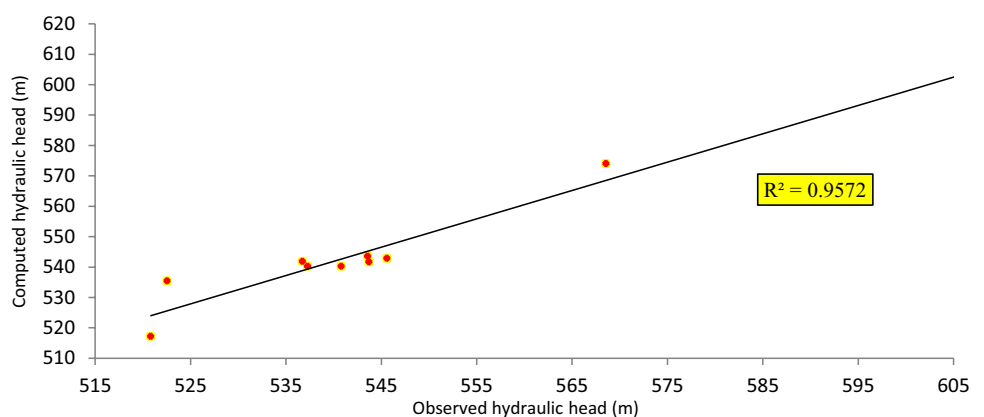
Horizontal <i>K</i> (m/d)	Vertical <i>K</i> (m/d)	<i>Sy</i>	Zone budget
62.0	6.2	0.12	1
174.0	17.4	0.22	4
0.17	0.017	0.23	5
180.0	18.0	0.1	3
112.4	11.24	0.25	2

for time steps of 31 days for the first 6 months during the year and 30 days for the second 6 months during the year.

3.2 Model calibration

According to the ASTM-D6033 [4] Standard, if residual values are a small part of the difference between the highest and lowest hydraulic head observed in the site (10% of this difference), the calibration process is correct for calibration of groundwater flow models. Since the minimum hydraulic head observed in Iranshahr aquifer scope is 523.40 m, and the maximum is 598.87 m, the acceptable amount of error for calibration was considered 7.55 m (Fig. 9). After steady-state calibration, the optimized value of the parameter “*K*” is determined using trial and error and automatic calibration through the PEST module and is recorded in Table 1. The calibration accuracy was very appropriate given the value of *R*² (approximately 96%) obtained by comparing the water level values calculated by the model and the measured values in the observation wells (Fig. 10). The optimized values of specific yield (*Sy*) are recorded in Table 1 after transient-state calibration of the model.

Fig. 10 Comparing the groundwater level (hydraulic head) values calculated by the model and the measured values in the observation wells



3.3 Particle-tracking model

In the particle-tracking model, a group of hypothetical particles is placed in a specific location, and their motion’s direction and time would be determined based on the water flow rate [33, 38]. By modeling the particle motion, their forward and backward motion could be simulated to determine the origin and destination of contamination [6]. Moreover, the wellhead protection area could also be determined over time, using the particles’ modeling [21, 22]. In this study, to model the contaminant transport path, MODPATH numerical code—which is a three-dimensional, particle-tracking, post-processing program developed by Pollock [32]—was used to determine the particle motion’s direction and time.

3.4 Backward particle tracking

Modeling of particle’s motion was used to investigate the origin of the contamination. In this modeling process, for determining the origin of particles received by the well, we modeled motion of particles from origin to the well. For this purpose, 20 particles were created in the center of 13 selected wells, and backward motion of particles was modeled for the periods of 10 (Fig. 11a), 100 and 1000 years (Fig. 11b, c). Due to the existence of fine-grained substance and clay sediments at some grains, the porosity of Iranshahr aquifer was determined as 0.2. The modeling results show that contaminant transport path in the selected wells of central plains adheres to the hydraulic gradient of the groundwater and is directed from the river to the wells in the westerly aquifer output and is the origin of contaminants. However, the direction in these wells is not quite the same as the previous direction, but in these wells, contaminant transport path is directed from the southern slopes of the mountains (west Iranshahr) to the western aquifer output. The difference can be attributed to the changes in hydraulic conditions in this part of the

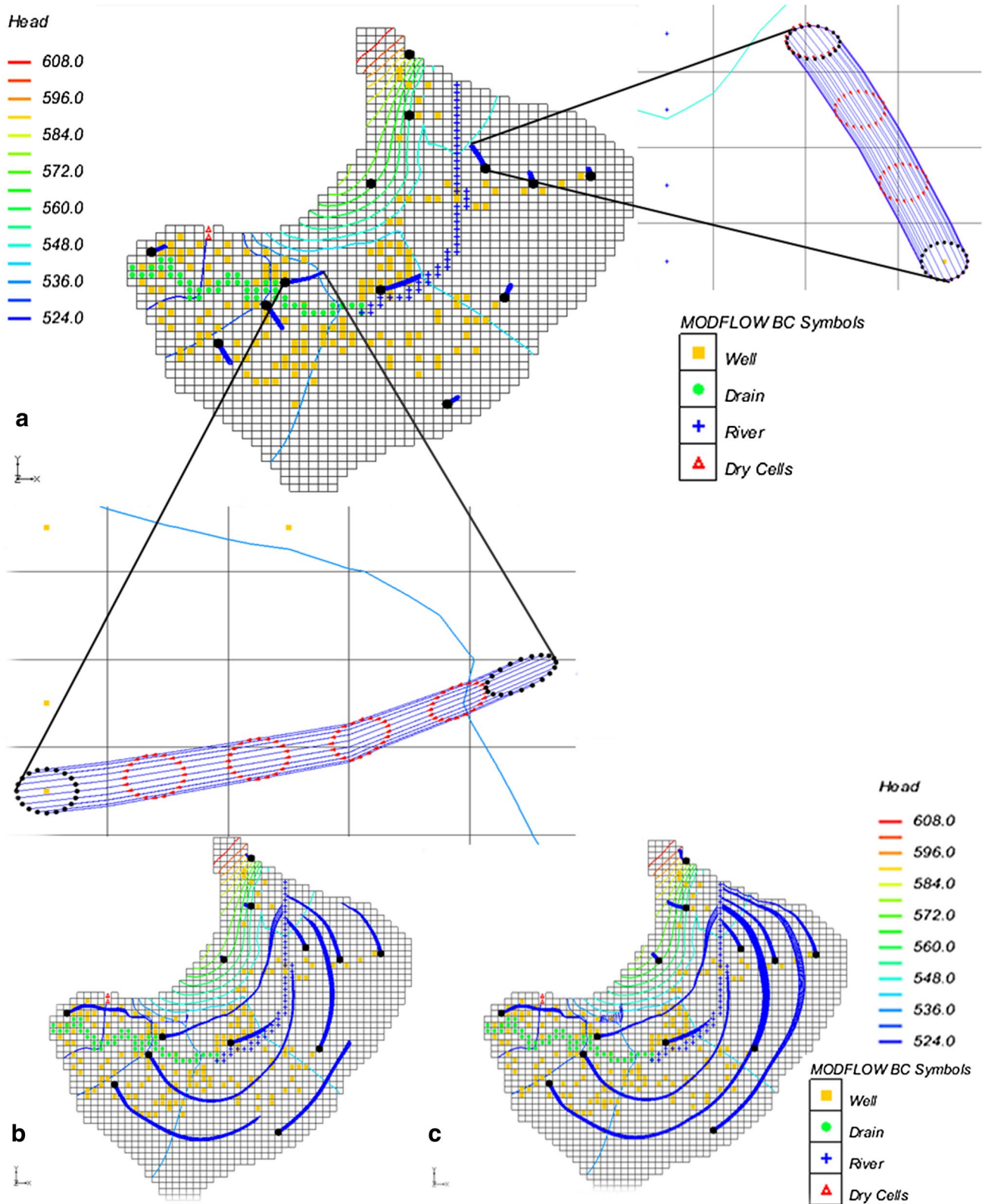


Fig. 11 a Modeling of backward tracking for selected wells, after 10 years; b, c modeling of backward tracking for the selected wells, after 100 years (b), after 1000 years (c)

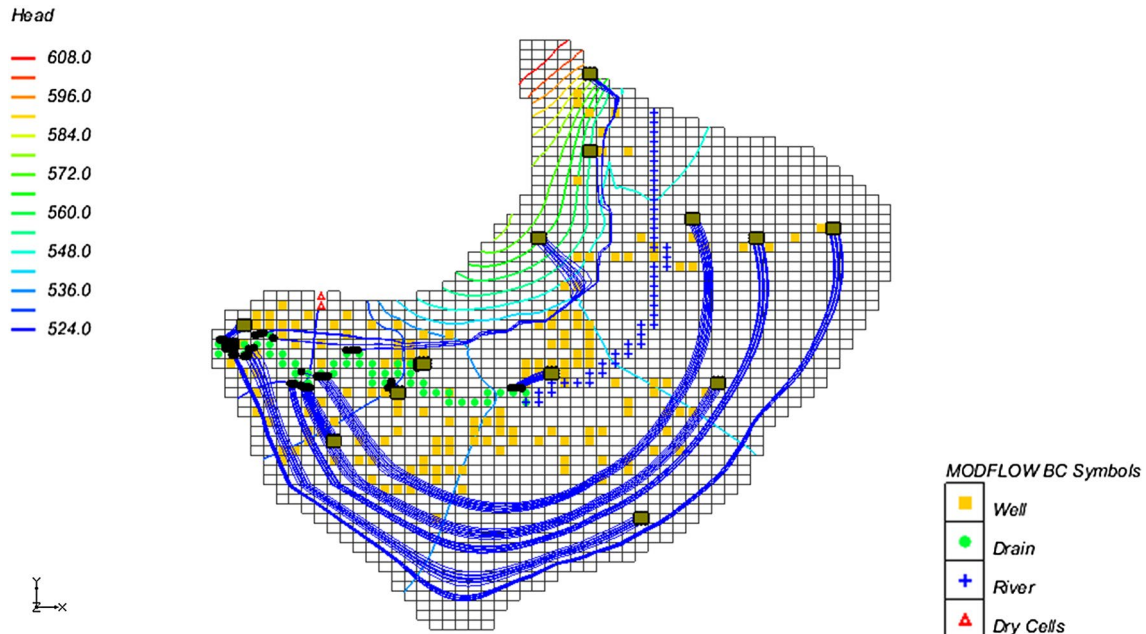


Fig. 12 Modeling of forward tracking for selected wells-track to end

aquifer and after drainage area because river changes into the drainage in these areas.

3.5 Forward particle tracking

Forward modeling of particle motion was used to study the path and travel time of the contamination. In this modeling process, for determining the travel time and path of particles in the well, we modeled motion of particles from well to the end of the aquifer in the groundwater flow path. As can be seen in Fig. 12, particle motion eventually exits from the aquifer after joining the drainage at the end western parts of the aquifer. The modeling results show that the maximum time taken by particles is 508,952.5 days, i.e., about 1394 years, and the minimum time was taken is 144 days. Moreover, the maximum distance travelled by the particles is 42,219.3 m, and the minimum distance is 988.2 m.

3.6 Wellhead protection area

Another feature of particle motion modeling over time is wellhead protection area determination. The areas with a constant radius of 50 days can be used to protect the well against the direct entry of contaminants through surface runoffs or leakage from the reservoirs near the well [10]. Also, fifty-day departure time means that it takes 50 days until the contaminants released into the ground may reach the well from a point around it before disappearance. This time is important in terms of the removal

of pathogenic bacteria (including coliforms) [19]. That is because most of them do not survive in groundwater for more than 50 days. Thus, in the last section of this study, the fifty-day wellhead protection area all over the aquifer was modeled by the MODPATH module. Figure 13 shows this wellhead protection area in Iranshahr aquifer. As can be seen in Fig. 13, inter-well interference has caused an increase in the wellhead protection area around some of the wells. The reason for this phenomenon is the interaction between the radiuses of influence of the wells that are near each other.

Although the wellhead protection area can be modeled, especially for non-reactive soluble materials in the MODPATH module, the wellhead protection area modeling for soluble materials during motion is influenced by porous media processes such as advection and dispersion. They need to use another module to incorporate these processes while the MODPATH module lacks such a structure. To solve this case, GMS software developers have developed an MT3DMS module that contains porous media processes.

4 Conclusion

To model for the contaminant transport path and determining the wellhead protection area in Iranshahr aquifer, firstly, flow model was prepared and calibrated, according to the interaction between surface water and groundwater. For this purpose, ModFlow2000 module in GMS

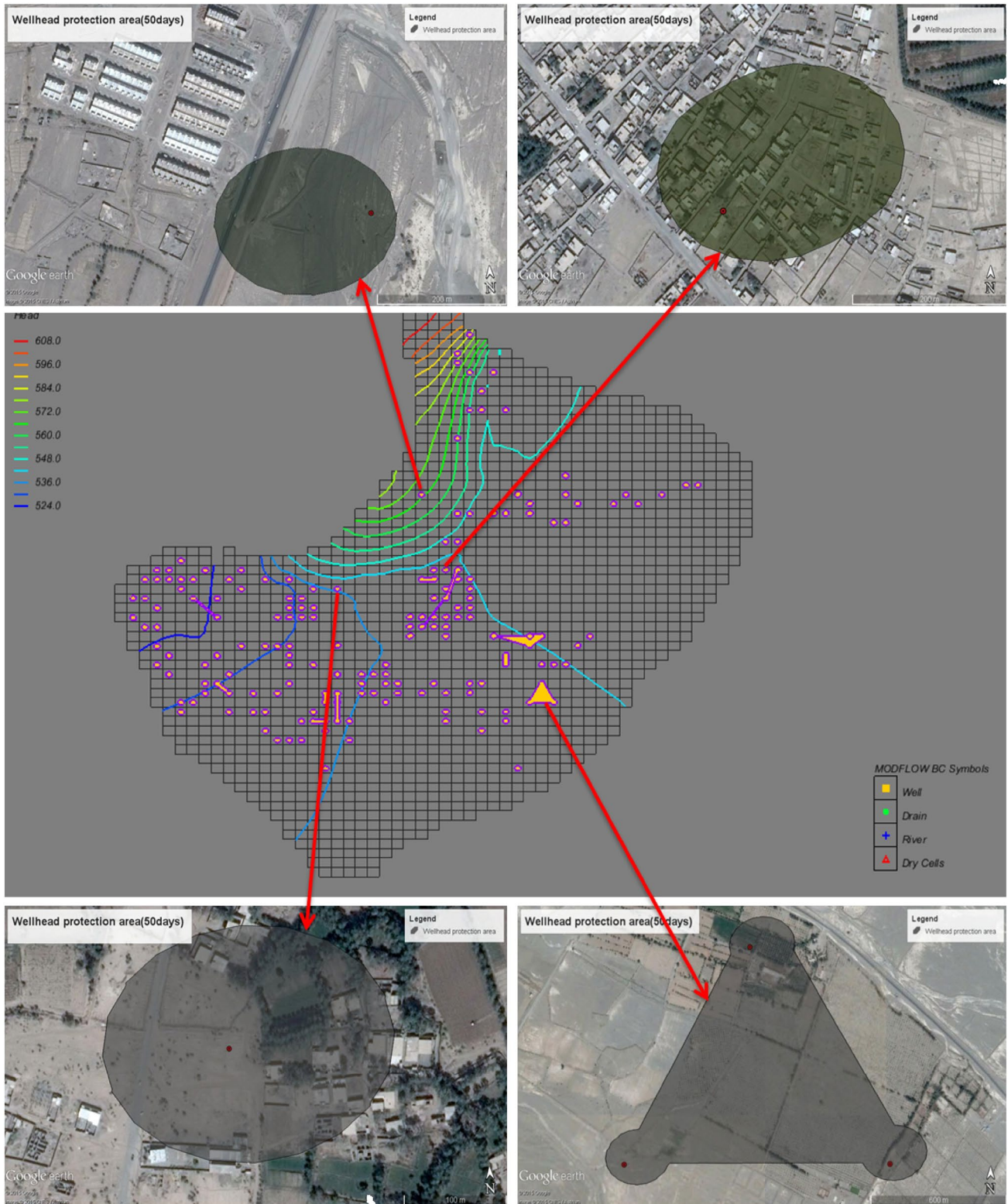


Fig. 13 The fifty-day wellhead protection area (light gray) of Iranshahr aquifer

software was used to develop the flow model, and manual and automated calibration procedures were used through PEST module for model calibration. Flow model calibration results showed perfect consistency between the observed and calculated groundwater levels with $R^2 \sim 95$. Based on the calibrated model, the highest hydraulic conductivity value was determined as 180 m/d (in the central aquifer), and the lowest was determined about 0.17 m/d (in the northwestern aquifer). Meanwhile, the specific yield value was determined between 0.1 and 0.25. After preparation of the flow model, contaminant transport model was developed using MODPATH module. Based on the results of this modeling, the origin of contamination in the selected wells is river in the northern aquifer, and some wells; it is the southern slopes of highlands in the east Iranshahr. Regarding the destination of contaminants, all contaminants in the wells ultimately led to the aquifer output drainage. Accordingly, the maximum time that particles travel along the contaminant path in the selected wells is 1394 years, and the minimum is 144 days. Moreover, the maximum distance travelled by the particles is about 42 km, and the minimum is less than 1 km. Finally, wellhead protection area was determined by model based on the protection against contaminations such as pathogenic bacteria. Accordingly, the average radius of wellhead protection area in Iranshahr aquifer was determined to be about 100 m.

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Compliance with ethical standards

Conflict of interest The authors declare that they have no competing interests.

Ethical standard It is confirmed that this manuscript is an original work of the authors and has not been published or under review in another refereed journal, and is not being submitted for publication elsewhere.

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