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Application of MODFLOW and MT3DMS Models to Evaluate Groundwater Quantity and Quality in Northern Iran

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Abstract

In recent decades, climate change and drought have led to an increase in groundwater use in the world. In Iran, due to being in the global dry belt and also the impact of climate change, reduced rainfall, and surface water, excessive use of groundwater, the amount of this valuable resource has decreased. According to groundwater changes, which have led to aquifer storage reduction, aquifers' evaluation is necessary. In this study, Haraz alluvial fan, located in the north of Iran, was studied using the GMS software, and the MODFLOW and MT3DMS models to simulate groundwater quantity and quality, respectively. MODFLOW is considered an international standard for simulating and predicting groundwater conditions and groundwater/surface-water interactions. MT3DMS can be used to simulate changes in concentrations of miscible contaminants in groundwater considering advection, dispersion, diffusion, and some basic chemical reactions, with various types of boundary conditions. The results of the MODFLOW model showed the maximum water level in the southern part of the alluvial fan at 125.07 m and the lowest in the northern part, adjacent to the Caspian Sea coast with -17.52 m. Also, on the MT3DMS model output, which was prepared based on Cl concentration, the maximum amount of this agent is 297.17 mg/L in the East and the northwest of the studied area. Management policy applied was the utilization of the alluvial fan aquifer within 2020 as much as the previous year. Model predictions indicated that the water level in piezometers increased by 0.75 m during 2021, and the maximum amount of Cl concentration remained unchanged. According to the results, it seems that the use of groundwater in the studied area is suitable for different purposes, considering climate changes and annual monitoring.

1. Introduction

The increasing population growth and rising living standards in many countries have necessitated higher-quality water resources for various uses including agriculture, industry, and drinking (Rahmani, 2010). Groundwater resources are valuable reservoirs, and understanding their capabilities and usage is considered essential infrastructure for developing countries (Mohamadi et al., 2011). From a global perspective, groundwater is considered for human consumption, supporting habitats, and maintaining the quality of base flow into rivers. Groundwater usually has excellent quality

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as it is naturally filtered through the ground, making it clear, colorless, and free of microbial contamination, requiring minimal treatment (Babiker et al., 2007). However, groundwater quality can vary significantly along its path, depending on factors such as path length and the abundance of soluble ingredients (Mahdavi, 2011). Due to the overexploitation of aquifers, many coastal regions around the world including the Middle East and North Africa, India, China, Japan, and Spain are encountering critical water resource sustainability issues (Llamas and Custodio, 2003).

Disputes among water users for groundwater rights have become common, particularly in highly exploited areas. The lack of knowledge about groundwater behavior hinders the formulation of suitable groundwater management plans. Mathematical modeling such as the use of models to simulate groundwater behavior can enhance understanding of aquifer conditions and resource availability (Bredehoeft and Hall, 1995; Bedekar et al., 2011; Doherty and Simmons, 2013).

Managing groundwater resources requires understanding aquifers in the first place and then predicting the effects of charging and discharging (Ghobadian et al., 2014). While long-term research is the best way to understand groundwater system behavior, it is costly and time-consuming. In the meantime, models can simulate groundwater systems with acceptable accuracy and achieve satisfactory results. The goal of applying an appropriate model is to simulate the real conditions of an aquifer using a series of mathematical equations. If a model is carefully applied, it can predict the future state of the groundwater system and clarify the impact of different conditions imposed on the aquifer, ultimately leading to the selection of a proper management strategy (Rahnama and Zamzam, 2013). One of these models that has many capabilities in simulating groundwater systems is the McDonald and Harbaugh model, also known as Processing Modflow for Windows (PMWIN), which was presented in 1998 and widely used by many researchers worldwide (McDonald, M. D. and Harbough, 1988). Stichler *et al.* (2008) estimated Lake Leis' contribution to pumping wells by simulating 18O 180 and 2H concentrations in the transient FEFLOW model.

Tritium concentrations in bores have been simulated with particle tracking MODPATH (e.g., Szabo et al., 1996; Pint et al., 2003; Bedekar et al., 2011; Hunt et al., 2006; Walker et al., 2007; Fienen et al., 2009; Starn et al., 2010; Eberts et al., 2012), but not enough work with MODPATH has been carried out on streams. MODPATH is a post-processing program that uses completely different mechanics of modeling tritium concentrations from MT3DMS (Pollock, 1994). In MODPATH, an adjective component of groundwater flow is considered that does not simulate concentrations; tritium concentrations are obtained by taking a convolution integral of transit time distributions. MT3DMS model, on the other hand, solves the transport equation in single- or dual-domain to obtain simulated concentrations. Based on the finite difference technique, leachate transport and penetration into the Hamedan Plain aquifer were simulated by exerting MODFLOW and MT3DMS codes in the GMS software. The results showed that the geological structure of the landfill area had the greatest influence on the development of leachate pollution of municipal solid waste in traditional disposal sites (Taheri Tizro, Sarhadi, Mohamadi, 2018).

Groundwater numerical modeling can be considered an effective tool for the sustainable management of limited available groundwater. Using the GMS: MODFLOW groundwater flow modeling software, the groundwater status in the Birjand region, southeast of Iran, was monitored. The results of the model were in good agreement with the observed data, and therefore, the model can be used for studying water level changes in the aquifer (Aghlmand and Abbasi, 2019). The groundwater level fluctuations of the Sonqor Plain are simulated by the GMS model, and the accuracy of the model is evaluated in two stages calibration and validation. Then due to the need for much less data volume in artificial intelligence-based methods, the GA-ANN and ICA-ANN hybrid methods and the ELM and ORELM models utilized groundwater level in Sonqor plain predict, instead of using the complex GMS model with a very large volume of data and also the very time-consuming process of calibration and verification. ORELM model has the best fit with observed data with a correlation coefficient equal to 0.96 (Khabat Star et al, 2022).

2. Materials and Methods

2.1. Study area

Haraz alluvial fan is limited to the Caspian Sea from the north and the Alborz Mountain range from the south. Amol and Mahmud Abad cities are located in this area. The region is located 36° 24 '5' 'to 36° 39' 40" north latitude and 52° 19 '5' 'to 52° 35' 9" East longitude and Haraz River is the main river in this place. The minimum height is -26.5 m near the Caspian Sea and the maximum height is 200 m in south of the study area (Fig. 1). 37 observation wells and 3166 operating wells are in the study area (Fig. 2) and the discharge of the wells is measured at 881775.5 million m^3 per year. Studied area geology includes coastline sand (QT2C) and farming areas los (QC) (Fig. 1).

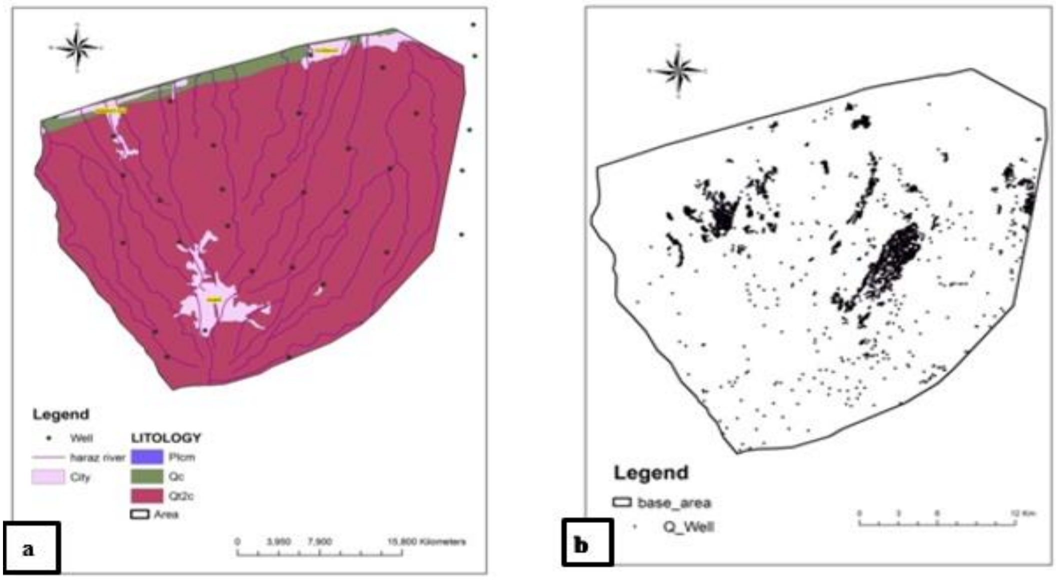

Figure 1. (a), Studied area with geology and position of wells and city (Amol, Mahmood abad, Sorkhrood). (b), Distribution of operating wells in Haraz alluvial.

Rainfall and the Haraz River, which feed (recharge) from snow and runoff of the Alborz Mountains, are the main water resources in the region. Geophysical reviews and exploration drilling are used for estimating alluvial thickness. Freshwater aquifer thickness in the Haraz alluvial fan is estimated over 300m (Regional Water Organization of Mazandaran Reports, Iran, 2012).

In this research work, several steps have been taken to approach the result; in Fig. 2, the research flowchart presents these steps.

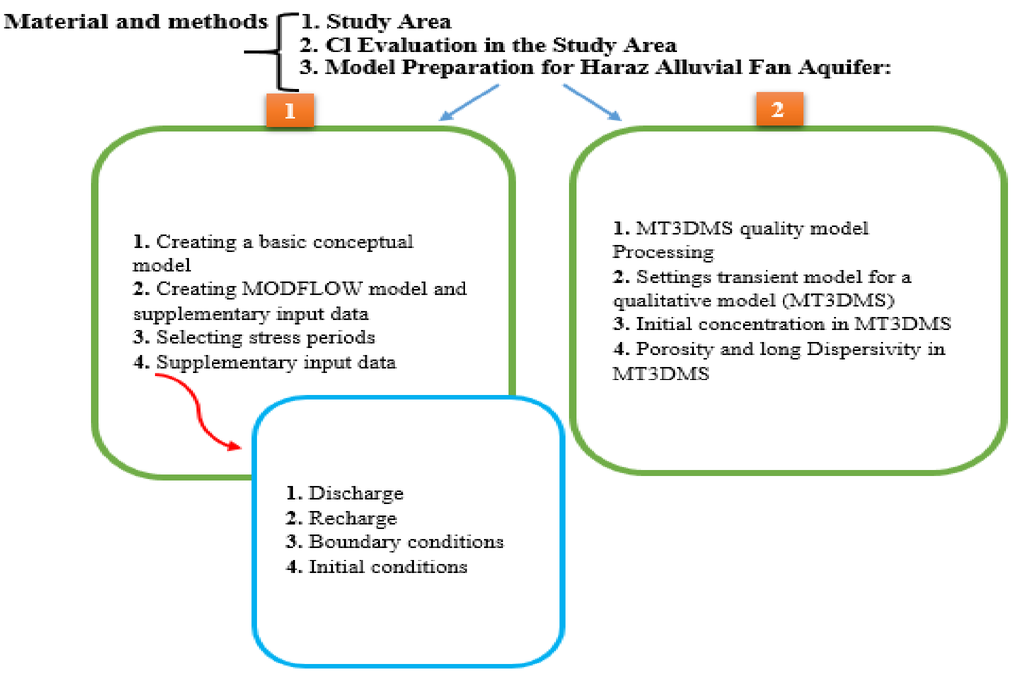

Figure 2. Research flowchart.

2.2. Cl evaluation in the study area

Cl (Chlorine) is measured twice in year in Iran, one in October and another in May; in the studied area, the amount of Cl in groundwater varies from 17–266 mg/L in October. Mapping Cl in October is due to occur minimum amount of rain from May to October, and during this period, groundwater level is low, agricultural return water is high, and Cl concentration is the highest in the year, and may represent the worst quality of groundwater in terms of the factor (Fig. 3).

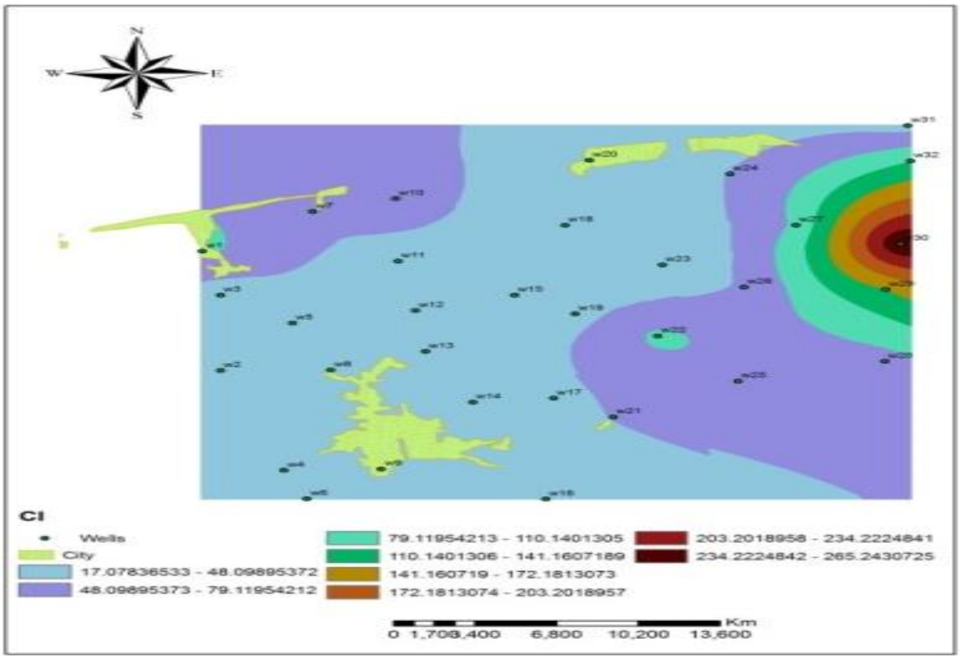

Figure 3. Cl map on September 2020 in Haraz alluvial aquifer.

2.3. Model preparation for the study area

In this study, the MODFLOW version (MODFLOW-2000) was selected to simulate three-dimensional groundwater flow. GMS7.1 is considered a graphical interface for the code (MODFLOW) and GIS database. Transient simulation usually needs to manage high volumes of data such as pumping wells data, recharge data, surface water level, and groundwater level in observation wells, collect, and organizing this type of information can be very boring. The GMS software was used because that provides a set of powerful tools for entering and managing data.

2.3.1. Model processing in GMS software for Haraz alluvial fan aquifer

- **Creating a basic conceptual model**

The conceptual model approach was used for creating a flow model in the GMS software. For this purpose, GIS tools and Map modules are used. At first model range must be specified in the image, and if specific boundaries are present such as borders with constant load (river), the boundary is defined in a separate cover. Sources/sink positions such as well position and surface recharge, layer parameters such as hydraulic conductivity and specific yield, model boundaries, and other information needed for the conceptual model are given to the software. After this step, the model network is created and the conceptual model is converted to a Grid model. 9 zones for hydraulic conductivity and 1 zone for specific yield were considered based on hydrogeology information (Fig. 4 (a, b)). The zones will be created in GIS, and then imported to GMS or produced directly in the GMS. The zones will be optimized in the calibration process.

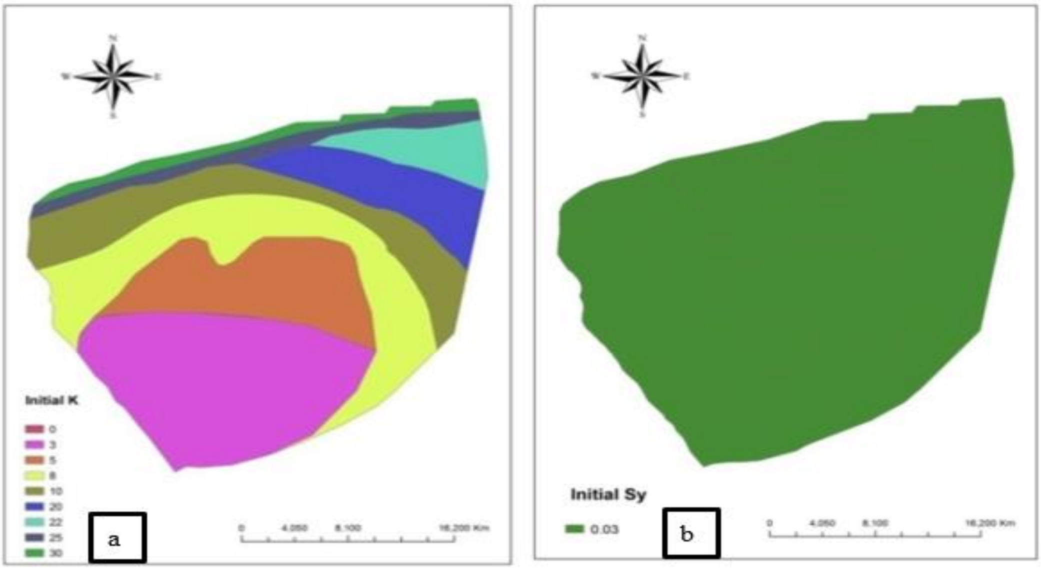

Figure 4. (a) Hydraulic conductivity initial zones, **(b)** Specific yield initial zone.

- **Creating MODFLOW model and supplementary input data**

To achieve this goal, at first, the grid frame location includes a determined network position and network navigation is found. Then three-dimensional network (3D Grid) was created. For the studied area, was designed a network with a 700 × 700 meters cell size including 47 cells in the vertical direction and 50 cells in the horizontal direction (3717 cells) and in one layer. In the next step, information on the upper and lower height of the layer and initial water level (September 2020) was entered into the model. Scatter points were used to apply surface topography and water level in the network cells that were entered into GMS by a text file, and then interpolated by facilities of software and automatically assigned to each cell. The surface topography can be seen in Figure 5. Surface topography data was imported to the model in a text file.

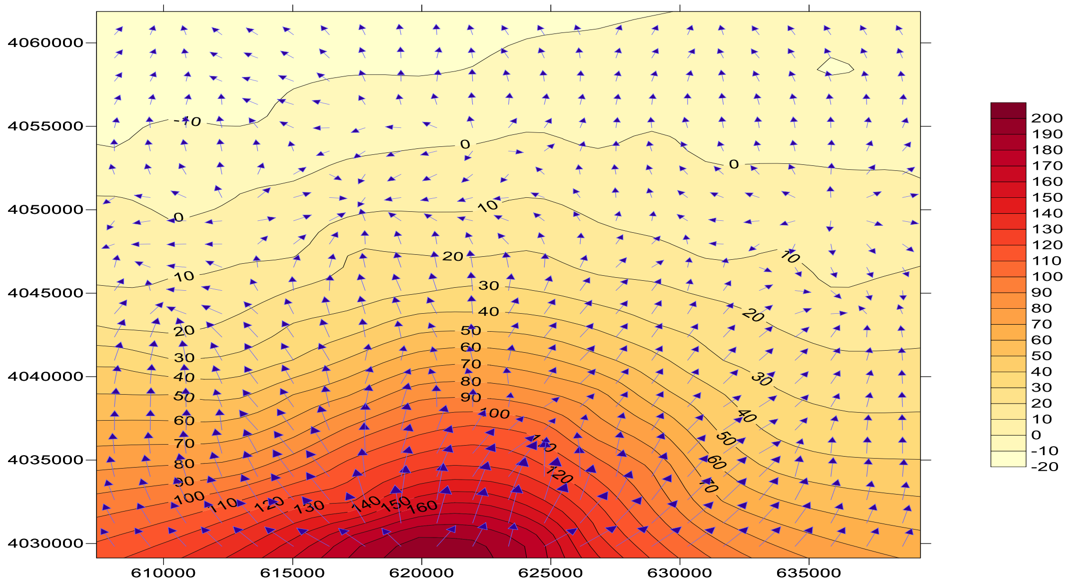

Figure 5. Topography and flow pattern in Haraz aquifer.

For beginning MODFLOW simulation, a conceptual model must be converted to a numerical model, then after the conversion, active and inactive parts of the model are determined automatically; finally, 1706 grid cells were considered active.

- **Selecting stress periods**

Because of aquifer transient conditions, the model should not be only run in stable conditions. Period and time steps were selected monthly based on available data for observation of water level. In total, 12 stress periods in one water year (2020) were considered to run the model.

2.3. Supplementary input data

2.3.1. Discharge

Water pumped by wells is the most important component of aquifer output, and in GMS is simulated in the discharge package. The volume of water extracted from the aquifer in 2020 was about 881775.5 million m^3 per year in the model range (Regional Water Organization of Mazandaran, Iran, 2007).

2.3.2. Recharge

The amount of surface recharge (including agricultural, drinking, industry, aquaculture, and precipitation return water infiltration) was simulated by the recharge package. According to the characteristics of the studied area and based on experts' opinions, the amount of return water was considered 20% for agriculture, 70% for drinking, industry, and aquaculture, and 10% for rain, and with regard to land use was applied in the model.

2.3.3. Boundary conditions

In the groundwater system choosing model boundary conditions is a very important step. In Constant Head Boundary (CHB), hydraulic load fixed throughout the boundary and for simulating aquifer boundary and surface water (rivers, lakes, etc.) is used (Batu, 2006). In the northern part of the model, the model boundary is adjacent to the Caspian Sea, thus this boundary is the General Head Boundary (Fig. 6). At the General Head Boundary (GHB), the input or output flow rate is calculated based on the difference between the hydraulic head in boundary cells of model and adjacent aquifer cells. Three packages in MODFLOW include of river package, drainage package, and GHB package can simulate these boundaries (Chitsazan, 2002). Based on the expressed description, the Northeast, Eastern, Southern, and Western boundaries of the model are General Head Boundary (Fig. 6).

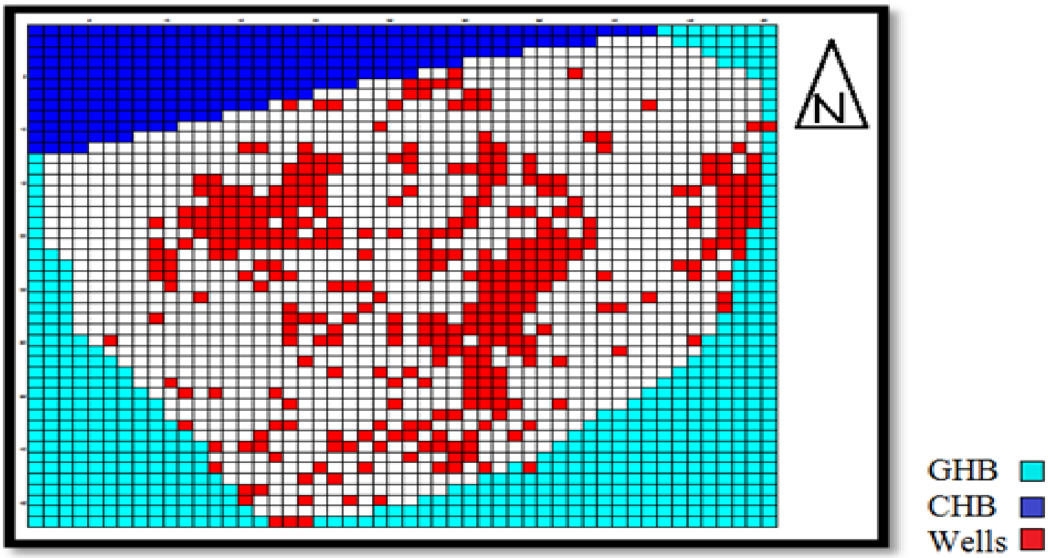

Figure 6. Haraz aquifer model boundaries (GHB: General Head Boundary, CHB: Constant Head Boundary).

Usually, the most uncertain component of groundwater balance is input or output flows. Haraz aquifer model boundaries, according to groundwater flow patterns, except in the northern part, are often seen as entrance boundaries in terms of hydrological (Fig. 6), the flows are the most important factor for aquifer recharge. The flow performance was simulated with the well package in GMS.

2.3.4. Initial conditions

Determining initial conditions are necessary to simulate transient condition. Groundwater level in September 2020 as the first water level was considered to start the simulation.

2.4. MT3DMS model

MT3D pollutant transport model was completed by Zheng and Bennett (1995). In recent years, different versions of the MT3D code have been used in the modeling of pollutant transport and groundwater assessment and clean studies. The new version of MT3D (MT3DMS) is able to solve transmission equations because the model has three methods in transmission equations in one code (standard finite difference method, Eulerian-Lagrangian method, and TVD method). MT3DMS and MODFLOW similarity in the structure of the program causes the MT3DMS selected model to easily be used in conjunction with MODFLOW (Zheng and Bennet, 2002).

2.5. MT3DMS quality model processing

In creating the qualitative model, at first, done a series of adjustments in the unsteady model (Transient), to get the result, and then Cl monthly data was entered into the model.

2.6. Settings transient model for a qualitative model (MT3DMS)

1. Set pollutant concentration units
2. Set MODFLOW to fit in MT3DMS
3. Model simulation
4. Select required packages for MT3DMS (Advection, Dispersion, Transport observation)
5. Set Stress period (Initial time step, Maximum time step, Maximum simulation time step)
6. Create porosity coverage and determine long dispersivity
7. Create Cl coverage
8. Run MT3DMS model

2.7. Initial concentration in MT3DMS

The most important parameter required in preparation quality models is the initial concentration of pollution sources, and as stated earlier; in this study, Cl was chosen. Cl is measured only two months a year in Iran; we imported only this data to MT3DMS. So, when interpolation is done in the model, it creates a high error, this error will decrease in the calibration process.

2.8. Porosity and long dispersivity in MT3DMS

Porosity and long dispersivity are as two most important parameters on model output. In the studied area were not measured these two factors, so at this point, this created new coverage in the model with name porosity. This coverage consists of long dispersivity and porosity. The coverage zoning was random (Fig. 7), after running the model the zoning was modified in the calibration phase.

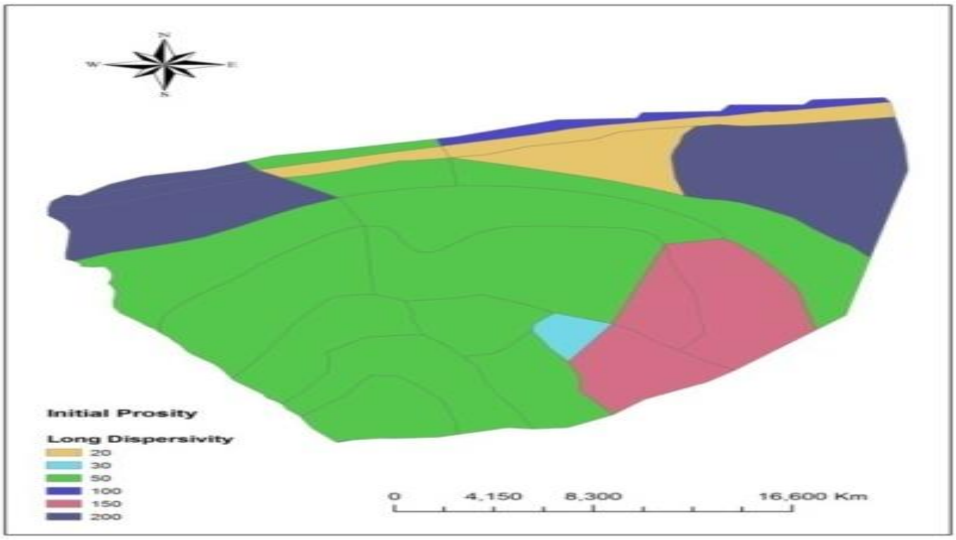

Figure 7. Porosity initial zones in Haraz alluvial fan aquifer.

After following the above steps, the model was run. The model's initial error (RMS) was 54.684, this error is modified in the calibration phase by changes in porosity and long dispersivity, and initial concentration of Cl.

3. Results and discussion

3.1. Steady state output

After calibration, the amount of error in most of the piezometers in steady state condition was less than 2 m in one stress period. Groundwater levels were determined by the model after its calibration in steady state (Fig. 8). As can be seen in this figure, the maximum groundwater level in the Haraz aquifer is in the south of the study area with 125.02 m, and to the north direction of the study area, the groundwater level is reduced to -17.52 m near the Caspian Sea coast.

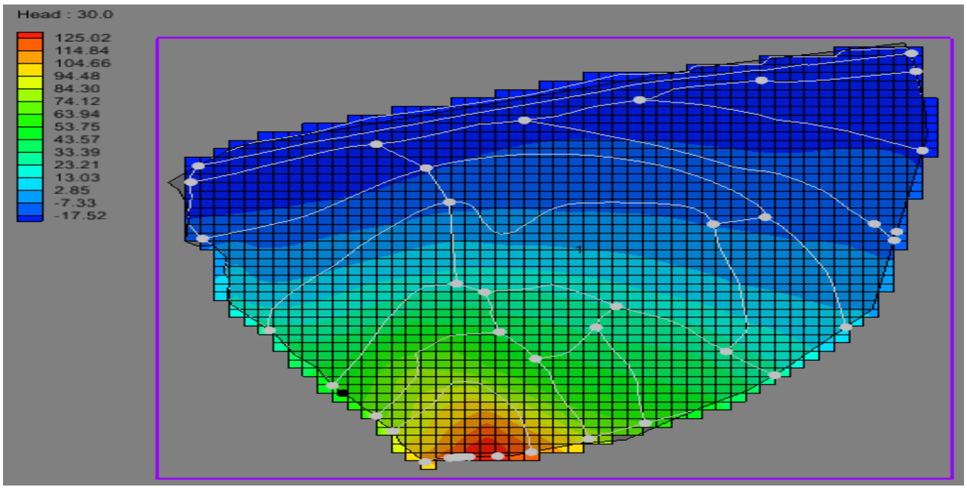

Figure 8. Groundwater level in steady state on September 2020 in Haraz alluvial fan aquifer.

3.1.1. Hydraulic conductivity correction in steady state

In fact, hydraulic conductivity indicates the soil component's connection status and water conductivity between two nodes. If the hydraulic conductivity (K) between two nodes is small, the connection between the two nodes is not good, in fact, there is an obstacle in the two nodes, also k correction is somewhat difficult and its value should be examined regionally. Figure 9 shows hydraulic conductivity zoning after correction. As you see, the studied area was divided into 16 zones in terms of hydraulic conductivity.

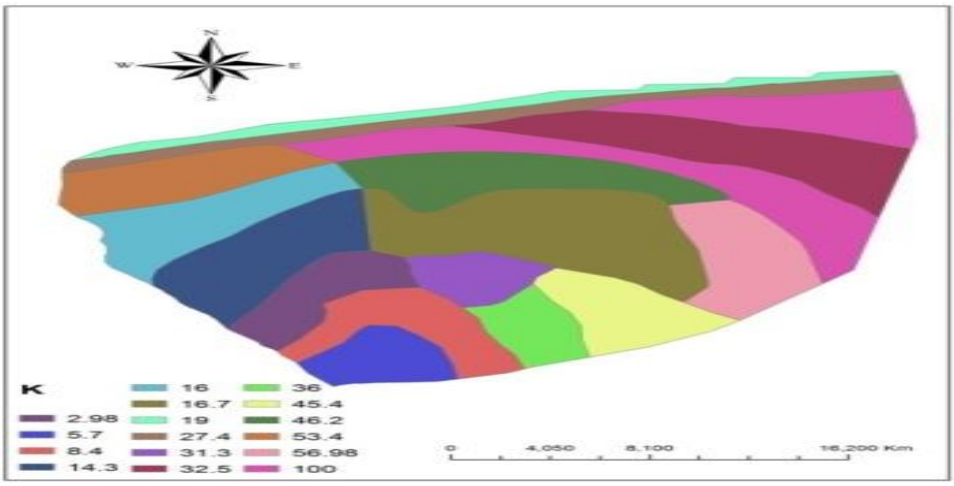

Figure 9. Corrected zoning of hydraulic conductivity after calibration in steady state in Haraz alluvial fan aquifer.

3.2. Unsteady state (transient) output

After calibration, the error in most of the piezometers in transient conditions was less than 2 m in 12 stress periods. RMS in transient condition was 1.975. Groundwater levels were determined by the model after model calibration in an unsteady state (Fig. 10). As you can see in this figure, the maximum of groundwater level in the Haraz aquifer is in the south of the study area at 125.02 meters, and to the north direction of the studied area, the groundwater level is reduced to -17.52 near the Caspian Sea coast. Figure 11 shows observations water level in the study area and the computational water level with the model in September 2020.

3.2.1. Specific yield correction in unsteady state (transient)

Specific yield impact in seasonal fluctuations of groundwater level in aquifer. In two places with the same conditions, if only the specific yield was different, water level fluctuations in the aquifer with a lower specific yield is further than aquifer with a higher specific yield. According to these changes, corrections were made for specific yield zones, and then new zoning was obtained after calibration, which is shown in Figure 12.

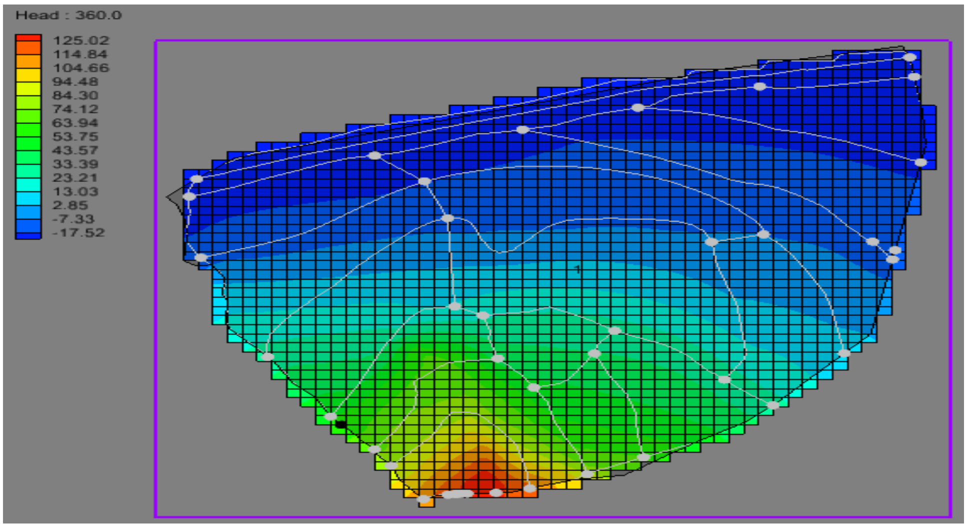

Figure 10. Model's computational water level in September 2020 in an unsteady state (transient) in Haraz Allu

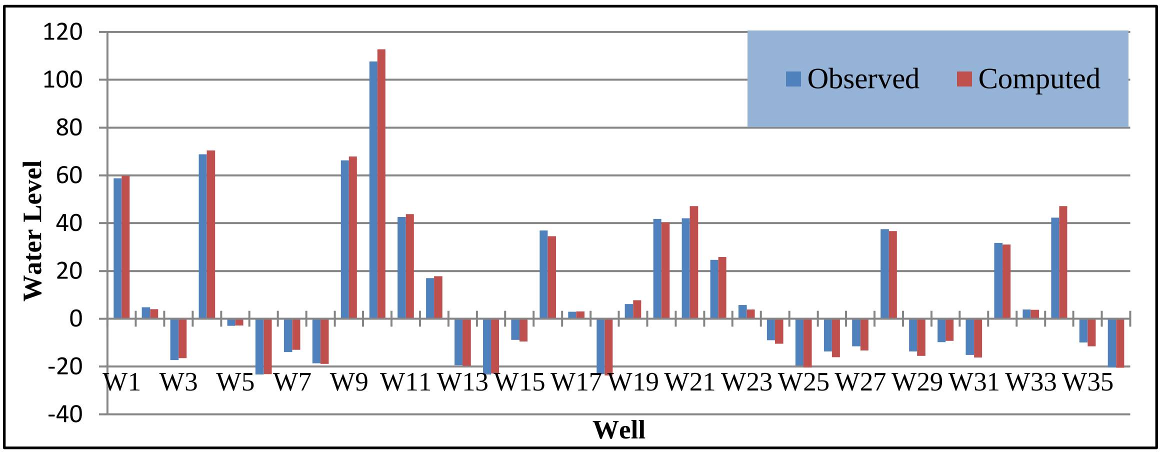

Figure 11. Comparison observed and simulated water levels in September 2020 for all wells in the Haraz alluvial fan aquifer.

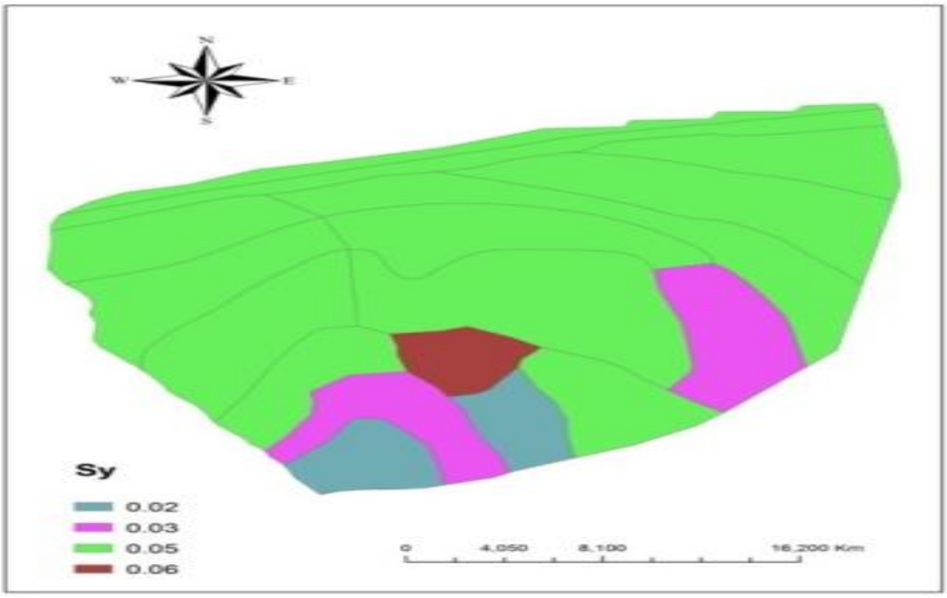

Figure 12. Corrected zoning of specific yield after calibration in unsteady state (transient) in Haraz alluvial fan aquifer.

3.3. MT3DMS quality model

3.3.1. Long dispersivity correction in MT3DMS

Long dispersivity in the groundwater pollution mathematical model is one of the effective parameters in model results. This parameter shows the capability of soluble dispersion in aquifer. Considering that determining accurately of this parameter accurately requires tracking tests and laboratory measurements. However, there have not been any track tests in the studied area. So, initially, this parameter was entered into the model randomly, and then it was corrected in the calibration phase.

At the beginning Haraz alluvial fan aquifer was divided into 6 zones in terms of long dispersivity, and after calibration, it was divided into 4 zones. Figure 13 shows long dispersivity zoning.

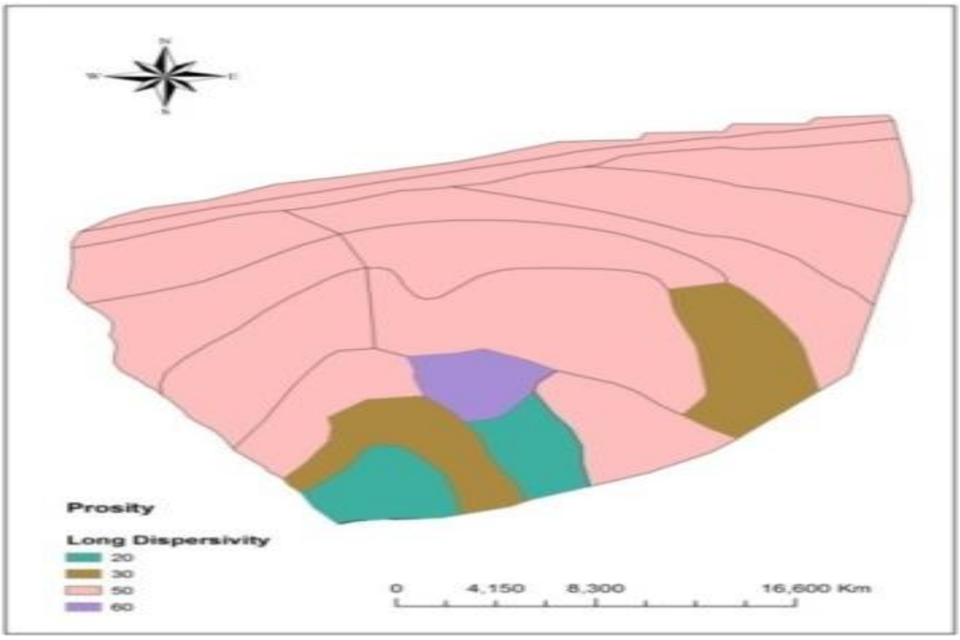

Figure 13. Long dispersivity zoning after calibration in Haraz alluvial fan aquifer.

3.4. MT3DMS quality model output

After quality model calibration RMS value reached to an acceptable level (before calibration RMS was 54.6 and after calibration, RMS was approximately 5). The amount of Cl in groundwater is measured twice each year; therefore, the error due to this factor is high, and reducing the error is very time-consuming in the model. Figure 14 shows the quality map output (Cl) in September 2020.

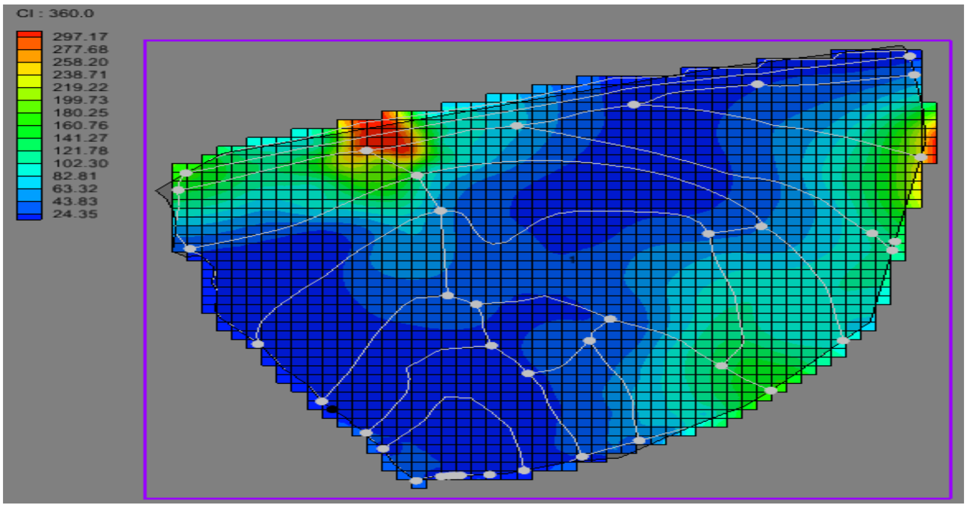

Figure 14. Quality model output on September 2020 in Haraz alluvial fan aquifer.

Quality model output in September 2020 shows that the maximum amount of Cl is northwest of the Haraz alluvial fan aquifer around Mahmoud Abad city with 297.17 mg/L, which is higher than the WHO standard (Cl < 250) (WHO, 2008), and similarly, in a small range of studied area in the east of the model Cl concentration reaches to 297.17 mg/L. The rest of the model range, which is a large area of the studied area, in terms of this factor was between 24.35 to 121 mg/L.

3.4.1. Management using MODFLOW and MT3DMS

Model is an efficient management tool for aquifer studies and hydrogeological and hydrological various stress studies. The model's unique characteristic is the ability to predict the future. By using models, the result of different strategies is visible with spending the least resources and cost. The main objective of preparing mathematical models for the Haraz alluvial fan is an assessment of quantity and quality changes in groundwater resources.

3.4.2. Strategies

The future status of the Haraz alluvial fan aquifer with the continuation current trend of using it. This strategy assumes that the current charge and discharge from the aquifer remain constant, and a decrease or increase in discharge or other specific changes are not done in the aquifer, and the aquifer status is to be evaluated in one year later (September 2021).

3.4.2. Groundwater level forecasting

Figure 15 shows the groundwater level in the Haraz alluvial fan aquifer at the end of the forecast period (September 2021). The piezometers position is shown in Figure 16. According to the model results, from 36 piezometers in the model range, piezometers number 4, 7, 9, and 10 have shown a drop in water level (14 cm), in piezometers number 2, 3, 5, 8, 12, 13.15, 17, 20, 22, 23, 24, 25, 26, 27, 28, 29, 30, 32, 33, 35, and 36 were observed relatively high water level rising (an average of 112.5 cm), piezometers number 1, 11, 14, 16, 18, 19, 21, 31, and 34 also show water level rising an average of 28 cm.

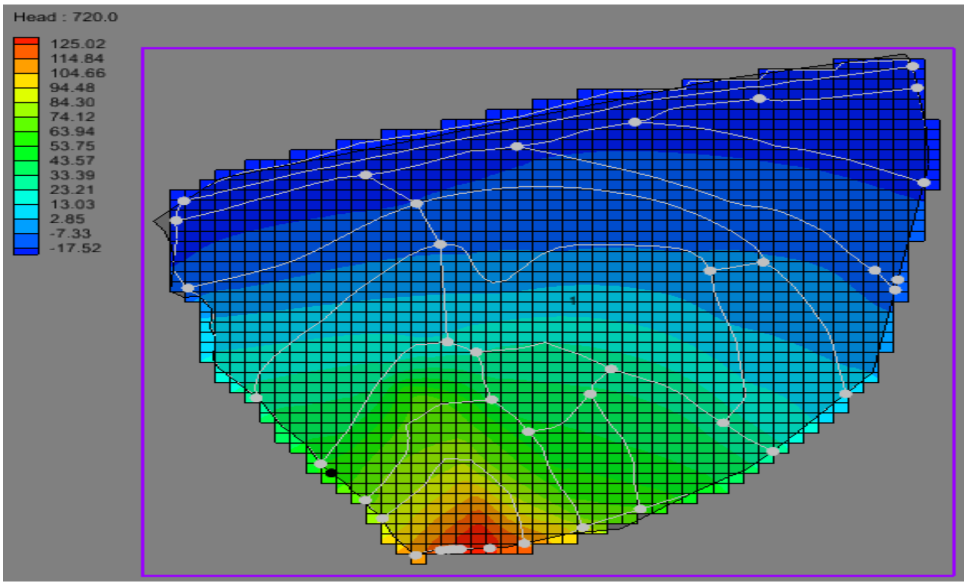

Figure 15. Groundwater level at the end of the forecast period (September 2021) in Haraz alluvial fan aquifer.

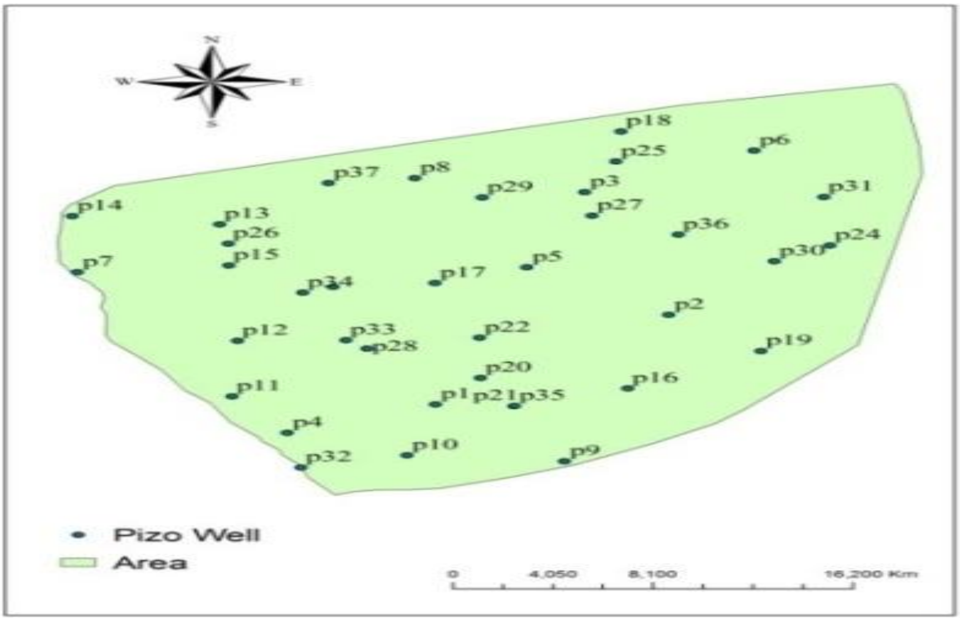

Figure 16. Piezometers position in Haraz alluvial fan aquifer.

3.4.3. Cl concentration forecasting

Figure 17 shows the Cl concentration in the Haraz alluvial fan aquifer at the end of the forecast period (September 2021). If uses of the aquifer do not change such as no change in charge and discharge, no change in number of utilization wells, no change in water level, rain similar to one year ago, and no change in other factors were entered into the model, the maximum amount of Cl is located in North West of Haraz alluvial fan aquifer near Mahmood Abad city with 297.17 mg per liter (Fig. 17) and in East of the study area with 297.17 mg per liter (Fig. 17), and it should be noted that this value of Cl is higher than WHO standard (WHO: Cl < 250 mg) (WHO, 2008). Cl concentration in a large part of the study area from North East to South West is in the range of 24 to 121 mg per liter (Fig. 17), this amount of Cl is less than the WHO standard amount of Cl.

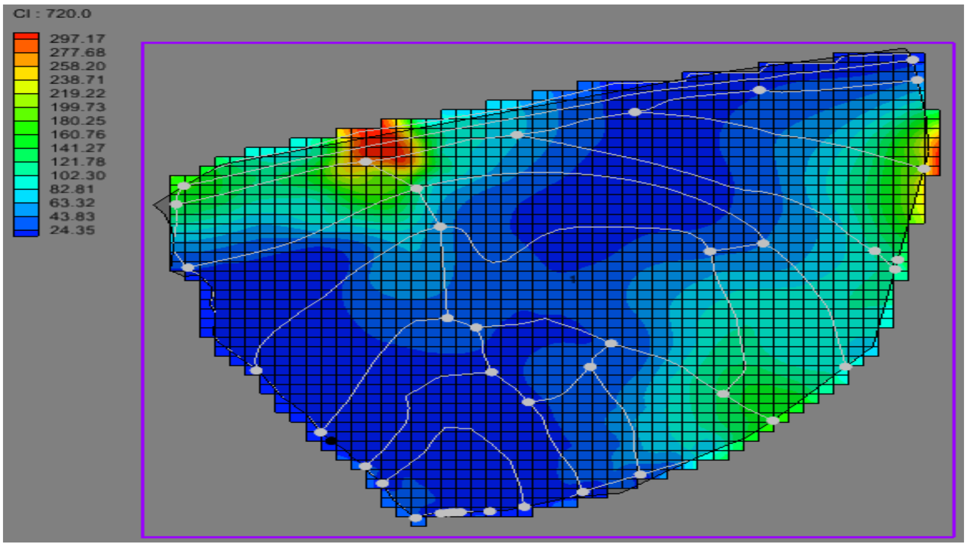

Figure 17. Cl concentration at the end of the forecast period (September 2021) in the Haraz alluvial fan aquifer.

4. Conclusions

Haraz alluvial fan aquifer is a one-layer and unconfined aquifer. The geological formations in the studied area include coastline sand and farming areas los. Sediment size decreases from south to north. The permanent river in the study area is the Haraz River, which emanates from the Alborz Mountains. In this study, to simulate the quality and quantity of groundwater in the Haraz alluvial fan aquifer, the MODFLOW-2000 version and MT3DMS version were selected, and modeling was done using the GMS software. The groundwater model in the Haraz alluvial fan aquifer includes a network with 700 × 700-meter cell size in one layer and includes 1706 active cells. There are 3166 operating wells and 36 piezometers in the studied area. The Haraz alluvial fan aquifer model was made in steady and unsteady states. The hydraulic conductivity in the steady state and specific yield in the unsteady state in the implemented mathematical model was reformed in the aquifer. After entering basic information into the model, the model was run in a steady state, and hydraulic conductivity was optimized. After reducing the error in the steady state, the model was run in the unsteady state. At this point, specific yield zoning was done randomly and then modified in the calibration phase. Cl data in September 2020 entered the MT3DMS mathematical model, and RMS was reduced to below 5 using the trial-and-error method. Groundwater level forecasting and Cl amount forecasting have been done for 12 months from September 2020 to September 2021. The management policy intended is the continued use of the aquifer from September 2020 to September 2021, like the past year, and its effects on the aquifer were evaluated by using the model. Anticipated results indicate an increase in water level in 22 piezometers, little change in water level in ten piezometers, and a reduction in water level in four piezometers. In total, the model predicted a 0.75-meter increase in groundwater level in September 2020 compared to September 2021. These results indicate proper recharge in the aquifer by river and atmospheric precipitation. These results also indicate that there is enough surface water for various activities, and there is no severe pressure on groundwater resources. MT3DMS quality model results indicated that Cl amount is between 24.35-297.17 mg/L in both September 2020 and September 2021 (forecasting period). The maximum amount of Cl is in the northwest of the model and on a small part of the model in the east, and this amount is higher than the Cl concentration standard (WHO: Cl < 250 mg/L) (WHO, 2008). The northwest part needs more attention due to the maximum amount of Cl concentration because it is located on the coast of the Caspian Sea, and there is a possibility of saltwater intrusion into coastal aquifers. The result of saltwater intrusion is degradation in coastal aquifers' quality. Reduced groundwater quality affected the region's plants. The optimal use of these resources can lead to the appropriate use of agricultural lands, and crop production will be guaranteed. That is an important step in a country's self-sufficiency and independence. Also, water quality reduction is likely to cause local people to migrate to another place for work and income. This leads to a serious social crisis in the future. In this research work, the lack of data in recent years did not allow us to construct a steady and transient model at present. Thus, the next step for this modeling is data collection in recent years for further studies. Nevertheless, in this research work, the hydraulic conductivity and specific yield zoning by the model in the studied area are very effective steps in the status of groundwater in the future. It makes that less cost and time will be needed in groundwater future studies in the study area. Finally, according to the results, it is suggested that the depth of bedrock should be determined exactly by using drilling logs. Because the depth of bedrock is one of the most important inputs of the model, and its accurate data existence will greatly help to facilitate conducting research. Also, because the amount of Cl in the groundwater in the eastern and northwestern parts of the study area is higher than the standard value, additional hydrogeochemical studies should be carried out to determine the source of salinity. Because the northern part of the model is the Caspian Sea coast, necessary studies should be carried out to determine the possible zone of saltwater intrusion towards coastal aquifers.

Data Availability

The data used to support the findings of this study is available from the corresponding author upon request.

Conflicts of Interest

The authors declare that they have no conflicts of interest regarding the publication of this paper.

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