Simulation of Mashhad Aquifer: A Successful Assessment Strategy to Control Groundwater Contamination

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Abstract— Identification of areas with heavy nitrogen loading from point and non-point sources is important for land use planners, environmental regulators and decision-makers. Once such high-risk areas have been identified, preventative measures can be taken to minimize the risk of nitrate leaching to groundwater. Most of the cities in the Third World countries face lack of wastewater collection systems which, in turn, could cause ground water contaminations. Elevated nitrate concentrations in drinking water can cause methemoglobinemia in infants, stomach cancer in adults and nitrate poisoning in animals as well. Modeling of nitrate fate and transport in groundwater to minimize nitrate concentration in groundwater has been studied by numerous researchers.

The present research focuses on modeling and assessment of Mashhad aquifer. The aquifer is serving most of the drinking water wells and its pollution threatens the health of city residents. A threedimensional numerical model was developed using PMWIN 5.3 to simulate the flow and transport of contamination in Mashhad aquifer. A total of 86 wells were selected for data collection from 2005 to 2012. The collected data showed that average amount of nitrate in observation wells was increasing every year. The increment is about 3mg/l per year. Average nitrate in observation wells in 2012 stood at 65mg/l, which exceeded the World Health Organization's (WHO) maximum contaminant level of 50 mg/lit for nitrate concentration in drinking water. The simulated and observed measured data showed that the model was able to predict the ground water quality changes within the aquifer.

Keywords- Modeling, Mashhad aquifer, Simulation, Nitrate.

I. INTRODUCTION

ROUNDWATER numerical Groundwater numerical J modeling has been widely used to simulate and predict the status of aquifers in recent years [1]-[4]. Comprehensive accounts of the behavior and application of numerical methods to groundwater problems have been discussed by numerous researchers. Bear [5], [6] used the basic equations of contaminant transport in groundwater. Abdel-Salam [7] applied a finite element solute transport model (CSU/GWTRAN) to a vertical cross-section in the Nile Valley of Egypt. Domenco and Schwartz [8] demonstrated the theoretical basis for the equation describing solute transport, which provided a conceptual framework for analysis and modeling physical solute transport processes in groundwater.

Khalifa [9] used a three-dimensional finite difference model (MODFLOW) to calculate future piezometric head levels and the total volumetric water budget for SiwaOasis project. Kolditz et al. [10] examined variable density flow and corresponding solute transport in groundwater. Farid [11] conducted a study to provide water quality guidelines to the Egyptian government. Dawoud [12] developed numerical simulation for transport of reactive multi-chemical components in groundwater.

William [13] used GIS system to analyze, interpret and manage the quality of groundwater and characterize the most vulnerable locations for contamination along the groundwater flow path between the capital city of Amman and Zarqa area in Jordon. Wang et al. [14] presented a numerical solution for equations describing advective-dispersive transport with multirate mass transfer between mobile and immobile domains. Bayer et al. [15] explained how to simulate source control with pumping wells located within the source zone. Bayer and Finkel [16] presented a comparison between pump-and-treat and funnel-and-gate systems as typical active and passive ground water remediation technologies. Schalk et al. [17] have proposed a modeling framework that takes advantage of the vast availability of measurement data in controlled water systems. Mohrlok et al. [18] analyzed experimental tracer transport in three-dimensional flow field for groundwater and subsurface remediation. Hamid et al. [19] presented a comprehensive evaluation of different finite difference schemes to solve head-based and mixed forms of the Richard's equation.

Most drinking water suppliers comply with the standard set by the World Health Organization [20]. Elevated nitrate concentrations in drinking water can cause methemoglobinemia in infants [21]-[24], stomach cancer in adults [25]-[27], and nitrate poisoning in animals [28]. As such, the US Environmental Protection Agency (US EPA) has established a maximum contaminant level (MCL) of 10 mg/l NO3-N [29]. In addition, consumption of nitrate-N has been linked to hypertension [30], disorders of the central nervous system, birth defects [31], certain types of cancer [32], [33], and diabetes [34].

Nitrate contamination in groundwater is a worldwide problem [35]-[40]. Nitrate is soluble and negatively charged and thus has a high mobility and potential for loss from the unsaturated zone by leaching [41], [42]. Previous studies conducted on the modeling of nitrate fate and transport in groundwater and on developing management practices to

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minimize nitrate concentration in groundwater can be classified into the following two broad categories: (i) studies that incorporated soil transformation models to determine nitrate leaching to groundwater [43]-[45], and (ii) studies that did not incorporate soil transformation models in the development of nitrate fate and transport models of groundwater [46]-[48]. Nitrate leaching from the unsaturated zone is the result of complex interaction among many factors (Fig. 1) such as the land use practices, on-ground nitrogen loading, groundwater recharge, soil nitrogen dynamics, characteristics of soil, and the depth to water table [49]-[52]. Accurate quantification of nitrate leaching is difficult as there are complex interactions among the land use, nitrogen loading, recharge, soil nitrogen dynamics, physical and chemical characteristics of soil, and depth of soil as indicated in Fig. 1 [53], [54].



Fig. 1. Schematic process of Nitrogen cycle [1]

II. STUDY AREA

The city of Mashhad with a population of 2.5 million is one of the most frequently visited cities in Iran. The city is located in Razavi Khorasan Province in northeast of Iran between Hezar Masjed and Binaloud Mountains. Mashhad plain extends between $36^{\circ}15'-36^{\circ}20'$ northern latitude and $59^{\circ}30'-59^{\circ}40'$ eastern longitude with an average altitude of 960 to 1,110m above the sea level. The current study area occupies 200km^2 with the average altitude of 980m above the sea level. Figure 2 shows the Mashhad plain.



Fig. 2. Mashhad aquifer relief map (2014 Google Maps)

Groundwater is one of the main sources of drinking water for the city. The contamination of groundwater is a major concern for municipal officials of the city. The burgeoning population and rapid growth of drinking water consumption has faced drinking water suppliers with more problems. The implementation of wastewater collection system has caused a drastic decline in groundwater level. Groundwater modeling was used to simulate Mashhad aquifer. Collected field data were used to calibrate and verify the model to predict groundwater status. Simulation techniques were used to assess the magnitude of the groundwater contamination with nitrate. To improve the groundwater quality of Mashhad residents, we proposed a few management techniques.

III. METHODOLOGY

In the current study, a transient, three-dimensional numerical model was developed using PMWIN 5.3 to simulate the flow and contamination transport in Mashhad aquifer. This program was originally developed for a remediation project at a disposal site in the coastal region of Northern Germany [55]. It supports MODFLOW and MT3DMS codes, which are widely used by researchers to simulate groundwater flow and solute fate [56]-[62]. PMWIN also uses PEST for inverse modeling which, due to lack hydrogeological data of aquifer, is essential in this study.

The three-dimensional movement of groundwater with constant density through porous earth material may be described by the partial-differential equation as follows:

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

Where K_{xxx} , K_{yyy} , and K_{zz} are values of hydraulic conductivity along the x, y, and z coordinate axes, which are assumed to be parallel to the major axes of hydraulic conductivity (*L/T*); h is the potentiometric head (*L*); W is the volume of volumetric flux per unit representing sources and/or sinks of water, with W < 0.0 representing flow out of the groundwater system, and W > 0.0 standing for flow into the system (T^{-1}) ; S_s is the specific storage of the porous material (L^{-1}) ; and t is time (T) [55]. A generalized partial differential equation describing the fate and transport of contaminants of species k in three-dimensional, transient groundwater flow systems can be formulated as follows:

$$\frac{\partial (nC^{k})}{\partial t} = \frac{\partial}{\partial x_{i}} \left(nD_{ij} \frac{\partial C^{k}}{\partial x_{j}} \right) - \frac{\partial}{\partial x_{i}} (nv_{si}C^{k}) + q_{s}C_{s}^{k} + \sum R_{n}$$

where C^{k} is the dissolved concentration of species k, n is the porosity of the subsurface medium, t is time, x_{i} is the distance along the respective Cartesian coordinate axis, D_{ij} is the hydrodynamic dispersion coefficient tensor, v_{zi} is the seepage or linear pore-water velocity, which is related to the specific discharge or Darcy flux through the relationship; $v_{zi} = q_i/n$, q_z is the volumetric flow rate per unit volume of aquifer representing fluid sources(positive) and sinks (negative), C_z^{k} is the concentration of the source or sink flux for species k, and $\sum R_n$ is the chemical reaction [56]. Hydrodynamic parameters of aquifer (transmissivity, specific yield...) are not measured in this area. The parameters were calculated in calibration process using PEST software.

A. Hydrological Setting

Collected data from 100 boreholes show that Mashhad aquifer is unconfined. Laboratory soil texture analyses indicate that in southern and western highlands of the city, soil texture is coarse while from south to north and west to east the texture gradually turns fine. Topography and bedrock of the aquifer are shown in figures 3 and 4, respectively.



Fig. 3. Topography of the Mashhad aquifer



Fig. 4. Bedrock of the Mashhad aquifer

B. Hydrochemistry

The main contamination source in Mashhad aquifer is domestic wastewater. Just as many other cities in Iran, lack of wastewater collection system has caused groundwater contamination in this area. Since most of drinking water supply wells are located in the urban area, drinking water contamination threatens the health of the population living in the city [63]. Domestic wastewater would leach into unsaturated and saturated layers of the aquifer. Although nitrate doesn't exist in domestic wastewater, it is produced and leach into groundwater through nitrification process. The measured nitrogen compounds analysis in Mashhad wastewater shows a concentration of 20 to 60 mg/l, which directly leaches into the Mashhad aquifer. To verify the model, 86 observation wells were selected. Average nitrate concentration in the observation wells was 42mg/l in October 2005 and 65mg/l in October 2012, which shows an average of %3 growth per year in contaminated Mashhad aquifer.

IV. MODELING

The Mashhad aquifer was assumed unconfined and singlelayer. Analyzing almost 100 boreholes has verified singlelayer assumption. In this area, there were 11 head observation wells available from 2005 to 2012. In modeling process, considering the extent of the area and available data, spatial discretization was done by dividing the model area into 37 rows and 45 columns, which made cells measuring 500 by 375 meter. The total number of cells was 1,665 including 1,219 active and 446 inactive cells. According to piezometric data of the aquifer, maximum and minimum groundwater level occurs in March and September. Therefore 14 time steps were defined for groundwater simulation scheme. The quantitative model was calibrated for the second half of 2005.

The assumptions for the aquifer recharge by irrigation for the first and second halves of the year were 25% and 50%, respectively. In addition, it was assumed that 60% of the consumed drinking water returns to groundwater in the first half of the year and 85% in the second half. According to the previous study in 1980 [63], infiltration rates of rain into the groundwater were considered 0.104 and 0.243 for the first and the second parts of each year, respectively. Authors have used the artificial piezometer method to enhance the model calibration accuracy. In the current study 133 artificial peizometers were selected (figure 5).



V. RESULTS AND DISCUSSION

Figures 6, 7 and 8 show the results of quantitative model calibration. Specific yield varied from 5.5% to 6% uniformly from higher to the lower part of the plain. Hydraulic conductivity distribution is also shown in figure 7 which varies from 5 to 35 m/day. Scatter diagram of observed head values vs. calculated head values are shown in figure 8. Results show a high correlation between calculated and observed head values. Verification of the model was performed using 2012 data. Figure 9 shows the simulated and observed groundwater contour map of this region in October 2012, which indicates the accuracy of the model for a seven-year simulation.



Fig. 6. Specific yield, Sy distribution of Mashhad aquifer



Fig. 1. Hydraulic conductivity distribution of Mashhad aquifer



Fig. 2. The Quantitative calibration of the Mashhad model



Fig. 3. The Quantitative verification of the Mashhad model

Calibrated model was used to predict the hydraulic heads in October 2020. Assuming the constant and current hydrological

conditions, average water level in the aquifer would decrease 11.5m by 2020. Figure 10 shows the drawdown distribution of the aquifer from 2012 to 2020. It shows that eastern parts had the drawdown between 1.5 to 5m and in the central parts the drawdown is between 5 to 15m. Maximum drawdown happened in Ghasemabad region which is more than 30m. Due to the lack of precipitations and also high density of extraction wells, drawdown would be more than 30m in western part of the Mashhad aquifer.



Fig. 10. Model prediction of hydraulic heads for 2020

In the current research, MT3DMS code was used for qualitative modeling. According to the Regional Water Organization data, amount of nitrate entering the aquifer is 7.75 gr/day/person in the study area. Figure 11 shows the nitrate contour map of the aquifer. This amount was applied to the model uniformly. By performing calibration process, the coefficient obtained was 0.00001cm3/gr. A total of 86 wells were selected to collect data from 2005 to 2012. A six-month average of nitrate measured data were used for calibration and verification processes. Figure 12 shows qualitative calibration of the model.



Fig. 11. The nitrate contour map of the aquifer



Fig. 4. Scatter diagram of qualitative calibration

Observed data show average amount of nitrate in observation wells has been increasing every year. This increment is about 3mg/l per year. Average nitrate in observation wells in 2012 stood at 65mg/l, which exceeds the WHO maximum contaminant level of 50 mg/lit for nitrate concentration in drinking water standards. [20].

To verify the model results and model precision, several years of measured data were used. Results showed that by increasing the prediction time, errors increase as well. The model could predict the concentration of nitrate in the aquifer only for 2 or 3 years accurately. Figure 13 shows the results of simulated and observed nitrate concentration distribution in verification process. The most important factor in increasing errors is the depths of observation wells in the area which varies from 100m to 250m. The extraction wells with the depth of 100m are more polluted compared to wells with a depth of 250m. The magnitude of pollution is depending on length and path of nitrate leachate.



Fig. 5. Comparison of model and measured nitrate concentration data

Calibrated and verified model was used to simulate and predict the nitrate concentration in Mashhad aquifer for the next 3 years. Nitrate concentration data in 2012 was used as initial nitrate concentration. Figures 14 and 15 show the nitrate concentration distribution for 2012 and 2015. Increasing water consumption and consequently increasing wastewater influx into the aquifer has caused the increasing nitrate concentration, except for the western part which has the wastewater collection system.



Fig. 6. The simulation of Nitrate concentration in 2012



Fig. 7. The simulation of Nitrate concentration in 2015

VI. CONCLUSION

To remediate degradation of water quality, the western part of aquifer should be recharged. A practical option is to use treated wastewater discharged by local treatment facility, recharged to the aquifer. Therefore, treated wastewater should be conveyed to the depleted region and artificial recharge plan should be performed. Also, simulation model shows that the precise nitrate contamination could be performed for the next 3 years. The model accuracy in central part of the area, which has the highest nitrate concentration, is low. This is due to high population density and possibility of high nitrate flux in central part of the aquifer. The procedure concluded in this study introduces the use of state-of-the-art computer simulation techniques for city managers to watch and predict consumed water quality. The simulation algorithm is proven to be an effective methodology.

ACKNOWLEDGMENT

The authors are grateful to Mohammad Rabbani for his technical and logistical assistance in data collection work, which was supported by authors. We also wish to thank Dr. Soori for technical help with modeling procedures.

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