

J. Environ. Treat. Tech. ISSN: 2309-1185

Journal web link: http://www.jett.dormaj.com



Modeling of Groundwater Quality for Drinking and Agricultural Purpose: A Case Study in Kahorestan plain

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Abstract

In the current study, planning for optimal utilization of groundwater resources is described. Kahorestan plain in Hormozgan province was the study zone. Since the main problem of the plain is high salinity of groundwater, chloride concentration was examined as an indicator of salt and also water quality degradations. This decision was made due to its high solubility, poor absorption, and stability of the compounds in the groundwater. A quality model was developed using software coding of visual mudflow to identify the problem. The collected chloride data of Kahorestan water wells were processed as an input in MT3D software from 2007 to 2011. Longitudinal and transverse diffusion coefficients were calibrated and the distribution of contaminants in the Kahorestan aquifer was analyzed. The mathematical model was developed to predict and simulate groundwater quality by October-2014. According to a developed qualitative model, the average concentration of chloride in groundwater was increased due to the need for more withdraw about a 5% increase in some parts of the northwest plains. Besides, the plain faces with a growth rate of chloride concentration about 3% compared to the initial situation in October-2011. Furthermore, to reduce the salinity, management schemes and plans were presented to reform water-use patterns, especially in the agricultural sectors.

Keywords: Groundwater, Salt, Chloride, Mathematical Modeling, Visual Mudflow

1 Introduction

Nowadays, Changes in the quality of groundwaters and salty water resources have been becoming the greatest warning to the agriculture industry, in particular, in arid and semi-arid lands. Therefore, many researchers have been doing to evaluate, estimate and measuring the concentration of contaminant properties either in fields or using a computation model [1-5].

Theorical foundations for describing the transfer of sakts, which is a conceptual framework to model analysis the modeling of the processes of transfering physical salts in underground water, was presented by Domenico and Schwartz [6] Khalifa, (1996) calculated the pizpmetric future levels and budget of water volume by a 3-D limited difference method for SiwaOasis project [7].

Lokman Hossain et al. (2013), investigated the status of

pond, supply, and tube-well water quality parameters (12 parameters such as pH, TDS, TS, SS, DO, COD, BOD, etc.) and identified water collection and distribution system in Chandpur district of Bangladesh. They found that all the parameters vary significantly with the types of water. Water quality management programs should be initiated under the supervision of the government to maintain the acceptable limit and proper water supply schemes should be followed for effective water collection and distribution systems [8].

Garba et al. (2016), evaluated 9 open well water contamination in the high-density residential area. Microbial contaminants, the concentration of some chemical and physical parameters were tested. The results showed that Nitrate exceeded the limit range in about 75% of samples while e- Coli bacteria were observed in 8 out of 9 samples. Overall, they recommended that another source of domestic

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water supply and other water purification techniques that is consumer-friendly is needed for the area [9].

Richards et al. (2019), investigated the spatial relationships between functional genes with chlorinated ethene concentrations in a surficial aquifer at a contaminated site by using cryogenic soil coring, and this result in that both aerobic methanotrophs and anaerobic VC-dechlorinators may play a significant role in VC biodegradation in aquifers that have little dissolved oxygen [10]. Panjaitan et al. (2018), used Chloride Bicarbonate Ratio Method to determine the seawater intrusion in the shallow aquifer by taking 30 samples with a 2 km distance each and measured Cl-, HCO3 -, CO3 - and EC as chemical parameters. The experiment showed that water usage debit and aquifer permeability affected seawater intrusion significantly with an adjusted coefficient R2 of 0.797 [11]. Banks et al. (2018), used the chloride mass balance (CMB) method to determine chloride decomposition in rainfall to estimate regional groundwater recharge in Africa. In order to provide input data for recharge estimation, simple rainfall collectors were developed and installed in sites, and also, other available researches data about chloride concentration in rainfall were used to create a regional map of chloride decomposition [12]. Xie et al. (2018), utilize an analytical model in three cases for contaminant transport in a vertical cut-off wall and an aquifer system. With a fixed hydraulic gradient of 0.5, the chloride (Cl-) breakthrough time increased by 1.7 which was more sensitive to the scale of the aquifer that the same trend of lead (Pb) [13]. Alexandria Demi (2018), considered the variation in groundwater geochemistry in the Great Bend Prairie aquifer by collecting samples from 24 wells and comparing results to previous data. Results demonstrated that water quality in the aquifer has degraded over the past 30 to 40 years due to nitrate accumulation [14]. Mountadar et al. (2018), studied the salinization mechanisms in the coastal area between Sidi Abed and Ouled Ghanem (El Jadida Province, Morocco) based on analyzing and discussing the physicochemical data of water samples from 73 wells. They found that the wells which were located in the coastal fringe are characterized by a high concentration of sodium and chloride and EC values but lower values were found in that of located in upstream, and the groundwater is contaminated by seawater intrusion [15].

Underground waters, is very important in Iran because of its dry climate. During the past 20 years, quick population growth, developing urban and agriculture areas, surface water restriction and overuse of underground water have led to serious damages to underground water aquifers in the country. Kahorestan plain in an important agriculture center in the west of the Hormozgan province which provides a portion of drinking water of Bandar Khamir and surrounding villages and also supplies the water requirement of the cement factory of the Hormozgan through the undergroundwater sources from its northwest part. Consequently, underground water quality has been decreased due to overusing [16]. Management of underground water in both forms of quality and quantity needs to be noted carefully. On the one hand, sources of contaminants and related equations should be well-known and on the other hand, advanced methods such as simulators and models with clockwork precision would better to be used to provide the most likely

conditions similar to what is in the reality and result in satisfactory outcomes [17]. The combination of chlorine, which considers in halogen categories, and sodium leads to produce salt. Serious kidney damages a high blood pressure are repercussions of increasing salt in drinking water [18, 19] and 20]. It is also might lead to stroke and left ventricular hypertrophy in a long-term period of consuming [21]. Some evidence has shown that consuming excess salt is an indirect reason for obesity with drinking soda [22]. It has been said that the risk of kidney stones, osteoporosis and one of the main reasons for gastric cancer are overusing salt [23 and 24]. Since the salt is the most soluble and the most extensive types of salt, it would be dangerous for the plants provided that there has not been an envolved mechanism to regulate its accumulation [25 and 26]. One of the predominant effects of chlorine on the human's health is disinfection by-product (DBPs) which define as side-substance that are produced in the presence of chlorine. This substance is caused by the reaction of chlorine and organic materials. Terly Halo Methane, Nitrozomines, and Halo acetic acid are the most important examples of DBPs that have great potential for cancer and genetic mutations in humans [27]. Hence, in the present study, we focused on the application of a quality model using software coding of visual mudflow to identify chloride concentration as an indicator of salt and also water quality degradations the problem. The collected chloride data of Kahorestan water wells was processed as an input in MT3D software from 2007 to 2011.

2 Methodology

2.1 Case Study

Khahorestan plain is located 90 kilometers away on the west of Bandar Abbas, and DMS latitude and longitude coordinates for Kahorestan are: 55°27' up to 55° and 27°8' up to 27°16'. Average altitude of the plain is 66 meters and almost 62 percent of the area is between 50 to 100 meters. Kahorestan plain is considered as the hot and dry areas with 156 millimeters average annual rainfall and 27°C average annual temperature. Average annual evaporation is about 3680 millimeters. Almost 60 of 260 square kilometer of the plain is suitable to be noticed and studied, and the rest is practically useless because of high salinity of underground (Laar Consaltant Engineering Company). Underground water flow modeling and soluble transfer

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

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial c}{\partial x_i} \right) - \frac{\partial}{\partial x_i} (V_i C) + \frac{q_s}{\theta} C_s + \sum_{k=1}^{N} R_k$$
 (2)

2.2 Ground water flow model and soluble transfer

Among the groundwater movement simulation programs, PMWIN and MT3D are more widely used due to the physical properties of the porous medium and their completeness. Most numerical models of groundwater are based on the solving of two differential equations with partial derivatives, which are the three-dimensional equations for the movement of groundwater with constant density in the porous medium, being explained as follows: $\frac{\partial}{\partial x} \left(K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{yy} \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_{zz} \frac{\partial h}{\partial z} \right) - W = S_s \frac{\partial h}{\partial t}$ (3)

$$\frac{\partial}{\partial x} \left(K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{yy} \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_{zz} \frac{\partial h}{\partial z} \right) - W = S_s \frac{\partial h}{\partial t}$$
(3)

In this equation, K is hydraulic conductivity, h is the potential load, W is the volume flux in the volume unit, which indicates the discharge and feed, S_s is specific storage for porous materials, t indicates time, and X, Y and Z represent the Cartesian coordinates [25 to 28]. The partial differential equations for transporting materials in a three-dimensional system in an underground aquifer are as follows:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial c}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (V_i C) + \frac{q_s}{\theta} C_s + \sum_{k=1}^N R_k$$
 (4)

where: C is the concentration of groundwater soluble contaminants, t times, x_i, the distance in the X direction in the Cartesian coordinate system, D_ij, the hydrodynamic relaxation coefficient, V_i the velocity of water in the aggregates, q_s the volume of the inlet or outlet in the unit that Inputs are positive and outputs are negative, C_s are the concentrations of inputs and outputs, θ are the porosity of the medium and $\sum_{k=1}^N R_k$ are the term of chemical interactions [29]. Three factors contributing to the transmission of pollution in groundwater include:

A) Advection: The contaminants in groundwater are transmitted according to Darcy law. According to the law, the flow rate from point 1 to point 2 is proportional to the head loss and has Photo ratio with the length of the path.

$$Q = -K.A.\frac{h_2 - h_1}{I} \tag{5}$$

The actual speed of passing through the soil pores is calculated as follows:

$$V = \frac{Q}{nA} = -\frac{K}{n} \cdot \frac{h_2 - h_1}{L} \tag{6}$$

where n is the Effective porosity or percentage of porosity that flow is passing through them. Therefore, only when the flow transfer is significant, the pollutant, along with the groundwater flow, does not move at the same rate and the concentration of the pollutant in the flow path will not be reduced.

B) Dispersion: Dispersion in underground waters actually indicates the spread of a contaminated substance in an area with groundwater velocity. The hydrodynamic diffusion coefficient is as follows:

$$D_L = \alpha_L V + \dot{D} \tag{7}$$

$$D_T = \alpha_T V + \dot{D} \tag{8}$$

where α_L and α_T are the longitudinal and transverse diffusion coefficient, V are the average water velocity of the groundwater and \dot{D} is the Effective molecular Dispersion coefficient.

$$R = \left[1 + K_d \frac{P_d}{n}\right] \tag{9}$$

C) Retardation: The process of delaying the movement of pollution in underground water due to the absorption mechanism, which is carried out both for organic particles and non-organic particles. The Retardation coefficient is calculated using the diffusion coefficients, absorption and soil porosity characteristics as follows:

$$R = \left[1 + K_d \frac{P_d}{n}\right] \tag{10}$$

where K_d is the absorption coefficient, P_d is the density of soil particles and n is soil porosity [35-36]. In this research, the quantitative model was first made, calibrated and validated by MODFLOW, then it was used to prepare a qualitative model. To provide a qualitative model of the MT3D package and the qualitative data of the 15 observation wells, chlorine measurements were used, as shown in Fig. 1. Due to the fact that we prepared and calibrated a small plain model for the years 87-88, we prepared a qualitative model for the year 2010 and we used the information from the following years to validate the model.

2.3 Predict the quantitative status of the aquifer in Kahurestan plain in Mehr (September- October: 2015)

In this section, a quantitative aquifer model is used to predict the level of aquifer water level up to 2015. In order to predict the future status of the aquifer, the level of water level in mehr October 2011 is given as the initial level of aquifer water level and is simulated for a 4-year period of aquifer.

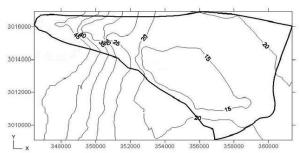


Fig 2: Forecast water level for October 2015

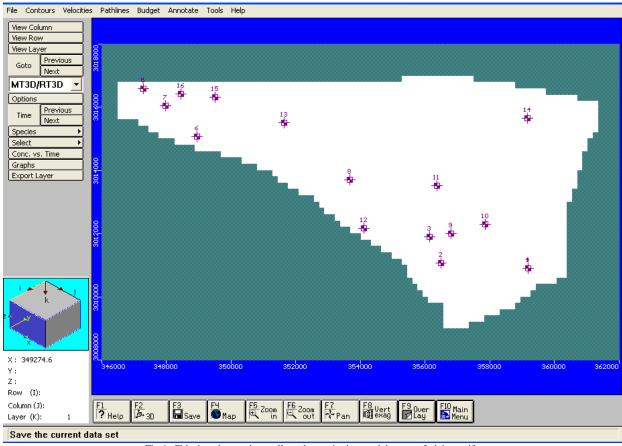


Fig 1: Chlorine observation wells and quantitative model range of plain aquifer

Figure 2 shows the distribution of water loss in the plain from mehr October 2011 to mehr September 2015 during a four-year period. As can be seen, using the quantitative model we conclude that the highest amount of water loss occurs in the northwestern part of Kahurestan plain.

2.3. Calibration of the model

In qualitative aquifer modeling, the parameters that are affected by the distribution process (absorption coefficient, horizontal distribution ratios to distribution length, vertical distribution to distribution length and distribution length) are calibrated. Basically, these parameters should be obtained from laboratory studies, but due to the lack of laboratory results data evidence, this was done by using trial and error and matching observational values with computational values. The calibrated parameters of the model are described in Table 1.

2.4 Error Distribution

Scatter diagram is a Comparison of the values calculated by the observation model as a graph. The distribution curve is, in fact, a kind of comparison of model results errors. Fig 4 shows the fitting of the results for the calibration period, which are acceptable with respect to the number of 15 observation plains wells. In addition, the qualitative model was calibrated for a one-year period. In Fig. 3, at the end of the calibration period, that is, after one year of simulation, two amounts of observed and calculated concentrations are compared.

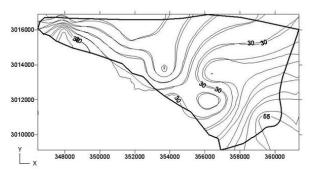


Fig 3: Lines map of calculated and observed Cl concentration in 365-day time step during the calibration period (2009-2008)

Table 1: The calibrated parameters of the model

TRPT	0.1	
TRPV	0.1	
DMCOEF	0	
Longitudinal Dispersivity	235	

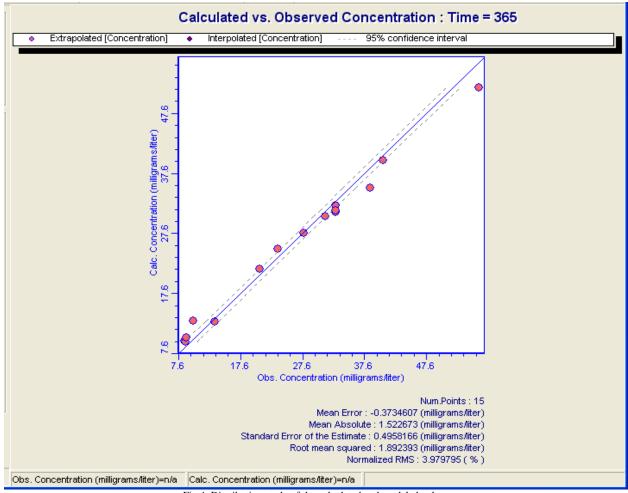


Fig 4: Distribution study of the calculated and modeled values

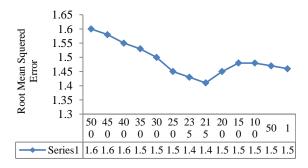
2.5 Parameters Sensitivity analysis

The purpose of the sensitivity analysis is to demonstrate the response of the quality model to the change of an unconfident input parameter. The model response to the variation of the input parameter can be high or low. The quality model of groundwater in Kahurestan Plain is sensitive to the length of distribution and the concentration of nitrate input and output of the aquifer respectively, and the model sensitivity to density of soil particles is low. Figure 5 shows the variation of the model error relative to the distribution length parameter.

2.6 Model Verification

To validate the model and determine the accuracy of it, the initial aquifer concentration was assumed to be the concentration for October 2007, and run the model for several consecutive time periods. The model results showed that the more predictive time goes, the greater the predictive error becomes. Based on the results, it can be said that it is quite obvious that maximum of 2 to 3 years to come can be predicted by this model and, for more than that, prediction accuracy becomes low, and is not recommended. Figure 6 illustrates this point and shows the accuracy of the model

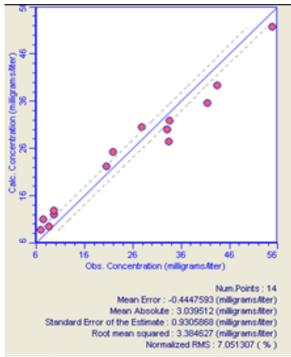
after 2 years (October 2009) and the accuracy of the model after 3 years (October 2010).



Longitudinal Dispersivity
Fig 5: Model sensitivity to diffusion coefficient

2.7 Predict

In this section, the model was used to predict the threeyear period. To do this, we initially considered the data of 2007 as the initial concentration and simulated the aquifer for a period of three years. As a result, the chlorine map in 2010 was shown in Fig. 7.



A: Model accuracy after 2 years (October 2009)

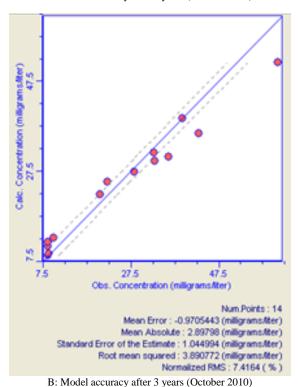
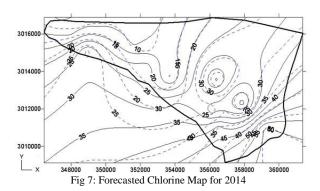


Fig 6: Distribution graph of observed and modeled chlorine concentration values



Then, in order to predict the chlorine concentration in the aquifer, the qualitative parameters in October 2011 as the initial values of concentration were given to the model and simulated for a 3-year period of the aquifer. In Figure 8, solid

simulated for a 3-year period of the aquifer. In Figure 8, solid lines of the map, are chlorine concentration lines in the October 2011, and dotted lines, are chlorine concentration lines in October 2011 Kahurestan plain.

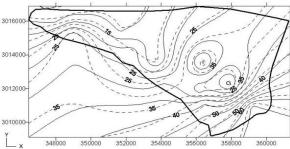


Fig 8: Forecasted Chlorine Map for 2014

3 Conclusion

In this study, PMWIN showed that it is a good option, both quantitatively and qualitatively, for the groundwater quality modeling of Hormozgan Plain. Modeling for the three-year forecast indicates that the amount of chlorine in the whole plain has a relative increase, which the average is 3.3% for the whole plain. This increase is due to more water harvesting in the northwestern plain. Thus, due to concidering the decrease in groundwater level, it is recommended to apply smart meter devices in these areas for efficient management of crop permitting, given the estimated water requirement of crops grown in the area and the methods of compensating for the loss of moisture.

The following two main axes can be examined. Long-term methods, including the proper use of modern irrigation and agricultural methods, are recommended and also necessary groundwater management changes in the area to compensate for groundwater quality. Short-term approaches include the creation of artificial feeding plans with regard to the potential of surface currents along the plain. This can be partially offset by a reduction in reservoir volume and improved groundwater quality. Therefore, by protecting water in agriculture by improving irrigation methods by taking steps such as problem solving and increasing the level of knowledge of farmers, developing an optimal cropping

pattern, preventing unauthorized harvesting and non-issuance of new licenses, protecting aquifers and artificial feeding. This can minimize the rate of groundwater level loss and its consequences.

Ethical issue

Authors are aware of, and comply with, best practice in publication ethics specifically with regard to authorship (avoidance of guest authorship), dual submission, manipulation of figures, competing interests and compliance with policies on research ethics. Authors adhere to publication requirements that submitted work is original and has not been published elsewhere in any language.

Competing interests

The authors declare that there is no conflict of interest that would prejudice the impartiality of this scientific work.

Authors' contribution

All authors of this study have a complete contribution for data collection, data analyses and manuscript writing.

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