Original Research Article

Validating Visual Modflow Numerical Model To Predict Future Impact Of Brine Disposal On Groundwater

ABSTRACT

The aim of this research was to simulate the brine disposal fate within an aquifer. The Visual MODFLOW numerical code was used to predict the salt concentration emigration over time in an aquifer. The model was calibrated using laboratory experiment data. The model results revealed that there is an acceptable agreement between the observed and simulated data.

Keywords: Desalination; Injection well; discharge well; salt concentration; aquifer

INTRODUCTION

Desalinated water is one of the non-conventional water resources where fresh water is produced from treatment of salt water. However, the negative impact of desalination process is the brine disposal which is a real environmental problem that should be considered and studied before constructing a desalination plant. The brine resulted from the desalination process is usually injected into aquifer or discharged into the sea. The practice of disposing the rejected brine into the sea is common for plants located in coastal areas [1]. The problem of disposing the rejected brine into the sea may increase seawater salinity leading to injuring plants and animals in the marine ecosystem [2, 3, 4]. In the case of disposing the rejected brine into the ground, it is necessary to design a disposal system in a way that respects the environment.

Numerical groundwater models have been used in developed countries since 1970's. Afterwards, there has been an increase in the usage of groundwater models, especially MODFLOW to address a wide range of water-related problems. The behaviour of production and injection well of desalination plants was assessed through an experimental setup and computational simulation [5]. Their results showed that the injection well will affect the salinity of the production well on the long run. The MODFLOW was used to simulate groundwater extraction for managing groundwater level in Jordan Valley [6]. A mathematical groundwater model for the Mahesh River basin in the Akola and Buldhana districts was developed using a MODFLOW model to predict the groundwater levels variation under different hypothesis conditions to manage the groundwater [7]. The MODFLOW was used to determine the interaction between the surface water and groundwater [8]. A mathematical model was developed for the Upper Awash river basin using the MODFLOW then calibrated it in order to manage the sustainable groundwater resource of the country [9].

Calibration/validation is a practice to ensure that a model represents the observed conditions of a studied phenomenon. Model calibration is the process where values of model inputs are adjusted so that the model matches the observed data [10]. In this research, the laboratory experiment of [5] is used to calibrate a model built with the Visual MODFLOW (VMOD) code. The main objective of this study is to simulate the fate of brine disposal within an aquifer using Visual Modflow software.

VISUAL MODFLOW MODEL

Visual MODFLOW is a software developed by Waterloo Hydro geologic. The software is used to simulate three-dimensional groundwater movement and solute transport. Visual MODFLOW provides many numeric engines that perform the numeric calculations required to solve the finite difference scheme of groundwater flow and mass transport. SEAWAT is the numerical engine implemented in this study as it simulates three-dimensional, variable-density, unsteady groundwater flow in porous media. The density-dependent groundwater flow model is governed by the equation developed by [11] as shown in Eq. (1)

$$\frac{\partial}{\partial x}\left(\rho K_{fx}\left[\frac{\partial h_f}{\partial x}\right]\right)+\frac{\partial}{\partial y}\left(\rho K_{fy}\left[\frac{\partial h_f}{\partial y}\right]\right)+\frac{\partial}{\partial z}\left(\rho K_{fz}\left[\frac{\partial h_f}{\partial z}+\left(\frac{\rho-\rho_f}{\rho_f}\right)\right]\right)=\rho S_f\frac{\partial h_f}{\partial t}+\theta\frac{\partial \rho}{\partial C}\frac{\partial C}{\partial t}-\underline{\rho} q_s \qquad (1)$$

Where ρ is the fluid density, K_{fx}, K_{fy} and K_{fz} are freshwater hydraulic conductivity in the x, y and z direction, h_f is the equivalent fresh water head, ρ_f is the density of freshwater, S_f is the fresh water specific storage, θ is the porosity, C is the concentration of solute mass per unit volume of fluid, q_s is the volumetric flow rate of sources or sinks per unit volume of aquifer and t is time. The governing equation for solute-transport is given by Eq. (2):

$$\frac{\partial(\theta C)}{\partial t}=\nabla(\theta D.\nabla C)-\nabla(qC)\pm q_s C_s \qquad (2)$$

Where:

D is the hydrodynamic dispersion coefficient tensor, q is specific discharge and

C_s is the solute concentration of water entering from sources or sinks.

NUMERICAL MODEL

Brine disposal by injection well in a coarse sand soil has been studied by [5] at Hydraulic Laboratory of Cairo University, Giza, Egypt using a rectangular seepage tank with dimension of 1.42 m long, 0.1 m wide and 0.4 m high. An injection well of 10 cm width was inserted on the left side of the seepage tank with a screen of 10 cm width that located at 0.15 m from the base of the tank. While, a constant head boundary is placed at the right part of the seepage tank with fresh water head 24.5 cm measured from the seepage tank bed represented by overflow vertical pipe screened at the upper end to prevent soil movement into the vertical pipe and opened at the lower end to drain excess water. A constant head reservoir containing brine water of 39,400 ppm concentration was used to feed the injection well at a rate of 0.144 m^3/day. Several observation points were constructed within the seepage tank to get the observed values of head and salt concentration as shown in Table 1. The head observed value and the salt concentration observed value at the specified location and time has been recorded by a sounder and a digital conductivity meter respectively. A numerical model was built to simulate the laboratory experiment using Visual MODFLOW as shown in the following section.

Models domain

As shown in Fig.1 the model domain consists of one row, 29 columns and one layer. Each cell, with the exception of the cells in column 1, is 0.05 * 0.05 m in size. Cells in column 1 are 0.02m * 0.05m.

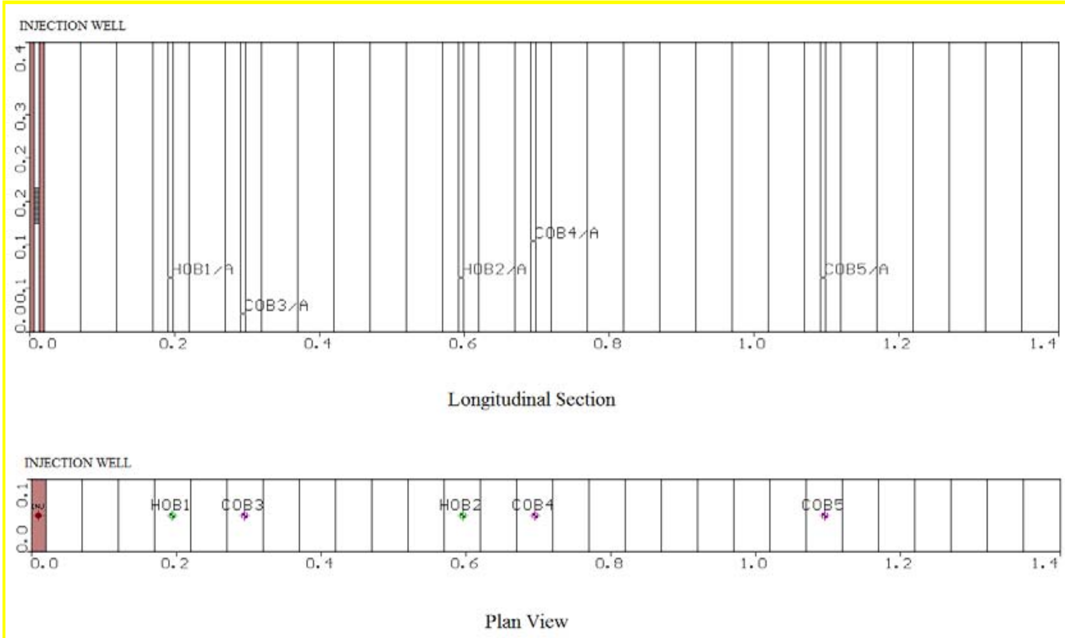

Fig.1. Model grids layout

Initial and boundary conditions

Initial NaCl concentrations in groundwater of the model domain are set to be 800 mg/l and initial fresh water heads are all set to be 0.245 m. Brine is applied in column one through a well (with a 0.05 m screen starting from 0.15m above the base of the seepage tank) with injection rate 0.144 m^3/day, and of concentration equal to 39400 mg/l. A constant fresh water head boundary of 0.245 m and a constant concentration equal to 800 mg/l are specified at column 29.

Model parameters

The parameters used in this model are hydraulic conductivity which is generally uniform and isotropic, specific yield, porosity and coefficient of effective molecular diffusion. The assigned values for these parameters were set to be 83 m/day, 0.27, 0.3 and $8.53*10^{-8}$ m^2/min respectively.

Observation Points

Several observation points were constructed within the model domain as shown in Fig.1 and Table 1.

Table 1. Observation points locations

Observation Point No.	Observation point type	X (cm)	Y (cm)	Z (cm)
HOB1	Head	19.5	5	7.5

HOB2	Head	59.5	5	7.5
COB3	Salt conc.	29.5	5	2.5
COB4	Salt conc.	69.5	5	12.5
COB5	Salt conc.	109.5	5	7.5

MATHEMATICAL MODEL CALIBRATION

In order to calibrate the numerical model, the initial and boundary conditions of the laboratory experiment were assigned. Injection well (injection rate 0.144 m3/day and of concentration equal to 39400 mg/l) and different observation points were represented in the model as specified by [5]. The records obtained from the head and concentration observation points are required during the calibration process of the Visual MODFLOW model.

Time steps were set to be 24 steps to represent both head and concentration values for 210 minutes (3.5 hours) simulation period.

Results of calibration

The laboratory experiment of [5] is used to calibrate the Visual MODFLOW (VMOD) model. The outputs of the model are illustrated in Fig. 2, Fig. 3, Table 2 and Table 3. A comparison between the results obtained from the VMOD and the laboratory experiment of [5] for the concentration observation points COB3, COB4 and COB5 is shown in Fig. 2 and Table 2. The correlation coefficient obtained from the model for these observation points were equal to 0.991, 0.995 and 0.981 respectively.

Fig. 3 and Table 3 shows a comparison between the results obtained from the VMOD and the laboratory experiment of [5] for the head observation points HOB1 and HOB2.The correlation coefficient obtained from the model for HOB1 equal to 0.901 and for HOB2 equal to 0.835.

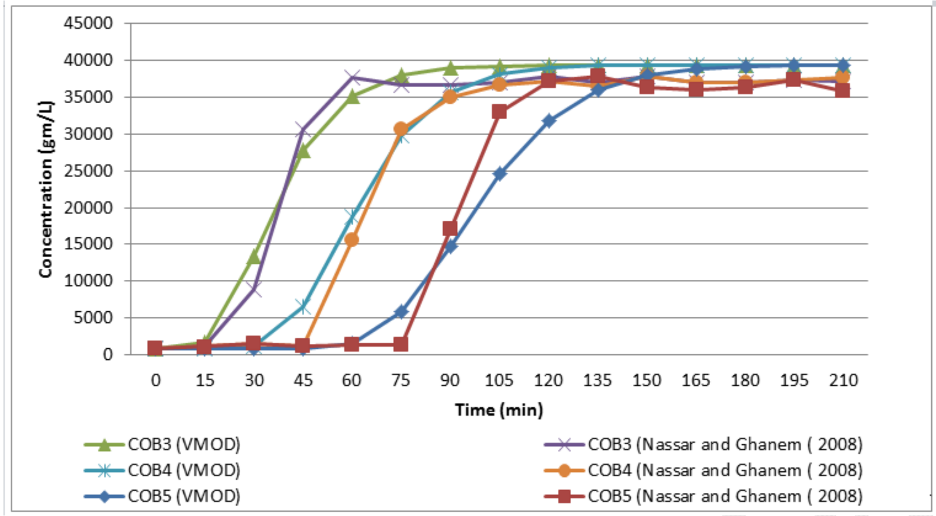

Fig.2. Comparison between results of Visual MODFLOW and laboratory experiment of [5] for COB3, COB4 and COB5

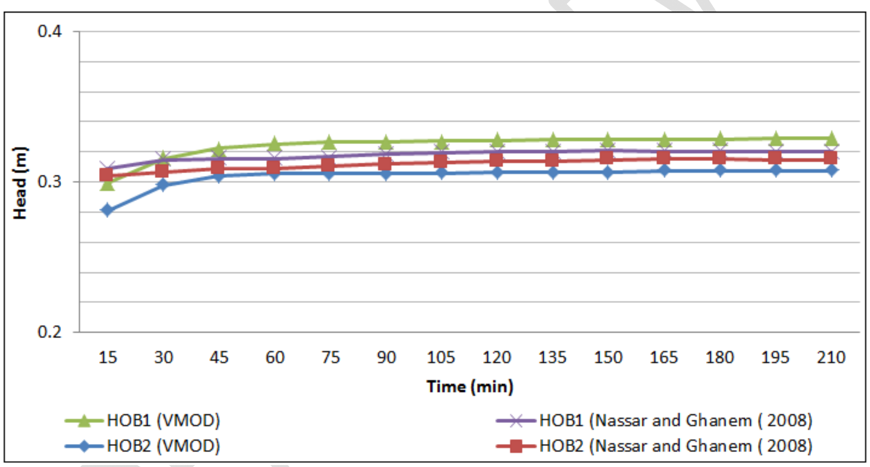

Fig. 3. Comparison between results of Visual MODFLOW and laboratory experiment of [5] for HOB1 and HOB2

Table 2. Comparison between results of Visual MODFLOW and laboratory experiment of [5] for COB3, COB4 and COB5

TIME (Min.)	COB3 (VMOD)	COB3 (Nassar and Ghanem (2008)	COB4 (VMOD)	COB4 (Nassar and Ghanem (2008)	COB5 (VMOD)	COB5 (Nassar and Ghanem (2008)
0	800	800	800	800	800	800
15	1711.6	1113.1	801.09	1113.1	800	1113.1
30	13460	8814.8	1262.5	1487	800.1	1487
45	27879	30623.1	6596.8	1254.3	832.52	1254.3
60	35129	37721.5	18843	15639.1	1600	1391.4
75	37937	36715.3	29842	30610.7	5805.3	1359.9
90	38926	36618.5	35669	34919.9	14708	17093.4
105	39255	36940.1	38087	36618.5	24597	33015.8
120	39362	37882.4	38975	37201.6	31828	37201.6
135	39392	37056.3	39271	36542.4	35943	37838.3
150	39397	37882.4	39363	37882.4	37951	36349.7
165	39398	37056.3	39391	37056.3	38832	36062.6
180	39398	36983.3	39399	36983.3	39192	36395.6
195	39398	37271.5	39401	37271.5	39329	37271.5
210	39398	37145	39401	37706.8	39378	35884.9

Table 3. Comparison between results of Visual MODFLOW and laboratory experiment of [5] for HOB1 and HOB2

TIME	HOB1 (VMOD)	HOB1 (Nassar and Ghanem (2008)	HOB2 (VMOD)	HOB2 (Nassar and Ghanem (2008)
15	0.2995	0.3088	0.2809	0.3041
30	0.3155	0.3148	0.2980	0.3065
45	0.3223	0.3156	0.3042	0.3089
60	0.3253	0.3155	0.3055	0.3089
75	0.3265	0.3166	0.3056	0.3103
90	0.3270	0.3183	0.3057	0.3118
105	0.3274	0.3192	0.3059	0.3127
120	0.3277	0.3202	0.3063	0.3136
135	0.3280	0.3201	0.3066	0.3135
150	0.3283	0.3211	0.3069	0.3145
165	0.3285	0.3206	0.3071	0.315
180	0.3287	0.3206	0.3073	0.315
195	0.3288	0.32	0.3074	0.3144
210	0.3288	0.32	0.3075	0.3145

Visual MODFLOW APPLICATIONS

It is important to design a discharge system for brine disposal that respects the environment and predict its effect on groundwater quality. Visual MODFLOW was used to detect the impact of brine disposal on the groundwater salinity by simulating four scenarios on the virtual aquifer as discussed in the following section.

Virtual coastal area

The dimensions of the virtual coastal area are 2500 m long, 1500 m wide and 150 m height as shown in Fig. 4. The groundwater level is at 50 m below ground surface and the aquifer thickness is 100 m. The east boundary of the aquifer **(**column 125**)** is the sea of concentration equal to 40000 mg/L. The discharge well is assigned at a fixed location 1020 m from sea, with a fixed discharge rate of 1200 m^3/day and the injection well is located at spacing (*S*) from discharge well. The screen length of the injection well equal to 20m starting from 0 m above the base of the saline aquifer.

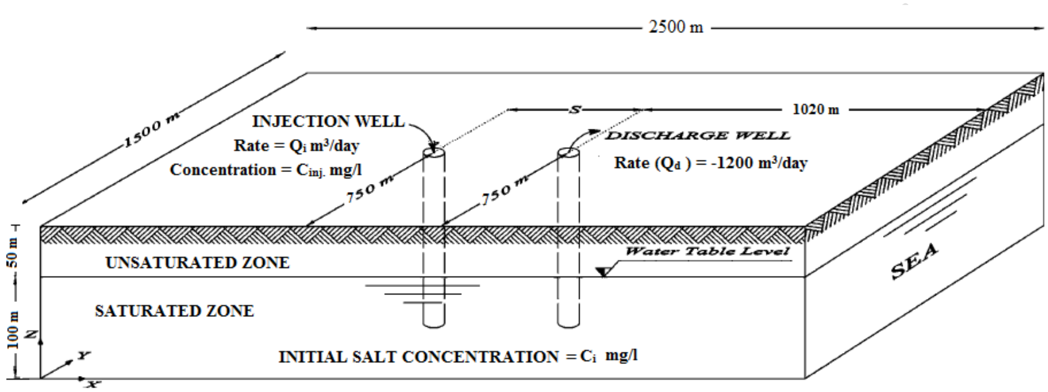

Fig. 4. Virtual coastal area layout

Where:

Q_{inj} : is the rate of the injection well,

Q_d : is the rate of the discharge well

C_{inj} : is the concentration of the injection well,

S : is the spacing between the injection and the discharge wells,

C_i : is the initial concentration of the aquifer.

Visual Modflow simulation

Visual modflow was used to simulate the density-dependent flow and mass transport of the virtual coastal area. The model domain consists of 75 rows, 125 columns and five layers. Cells of layer 2, 3, 4 and 5 are 20 m by 20 m in the horizontal, and 20 m in the vertical while, cells in layer 1 are 20 m by 20 m in the horizontal, and 70 m in the vertical. A general head boundary condition (GHB) was assigned along the outside edged of the model domain (column 1, row 1 and row 52) with conductance equal to 16 m^2/day.

The parameters used in the model were the specific yield, the soil porosity and the effective molecular diffusion with values 0.27, 0.32 and $1.228*10^{-4} m^2/day$ respectively. Concentration and head observation points were constructed within the model domain at row 38, column 75, and layer *k* (according to the screen location of discharge well) as shown in Fig.5. Ten time steps were used to represent both head and concentration values for ten years model run.

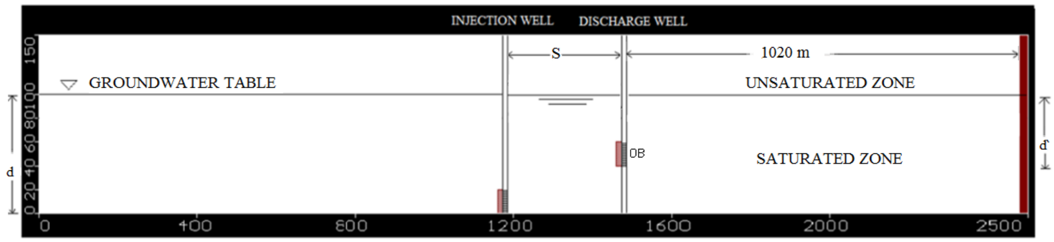

Fig. 5. Numerical model showing vertical layout, (cross section for row 38)

Where:

OB: is the observation point

d: is the location of the screen of the injection well from the water table

d`: is the location of the screen of the discharge well from the water table.

Simulated scenarios

In order to check the ability of the calibrated model in predicting the future impact of brine injection into the aquifer for different cases, four runs have been conducted as shown in Table 4.

Table 4. Simulated scenarios used in VMOD application

Scenarios	Initial conc. of aquifer (mg/l)	Injection Conc. (mg/l)	Q_d (m^3/day)	Q_i (m^3/day)	*S* (m)	*d`/d*
1	40000	80000	1200	600	100	0.6
2	40000	80000	1200	600	200	0.6
3	40000	80000	1200	600	300	0.6
4	40000	80000	1200	600	400	0.6

* is the hydraulic conductivity of the aquifer.

Application Results and discussions

The results of the simulated scenarios are shown in Fig.6 and Fig. 7.

Fig.5 is the design chart that has been developed by three design parameters, relative salt concentration (RSC), wells spacing (*S*), and simulation period (*T*). The Relative Salt Concentration at the discharge well (*RSC*) is given by Eq. (3):

$$RSC = \left(\frac{C_P - C_i}{C_i}\right) * 100 \qquad (3)$$

Where: C_P is the predicted concentration from VMOD, C_i is the initial concentration and *RSC* is the relative salt concentration.

Fig. 6 shows that after 10 years of simulation, as the spacing increases by 300% the RSC decreases by about 66%. So this indicates that the RSC is **inversely proportion** to the spacing between the injection and discharge wells, but we have to take into consideration the available area for constructing the desalination plant and the cost of construction.

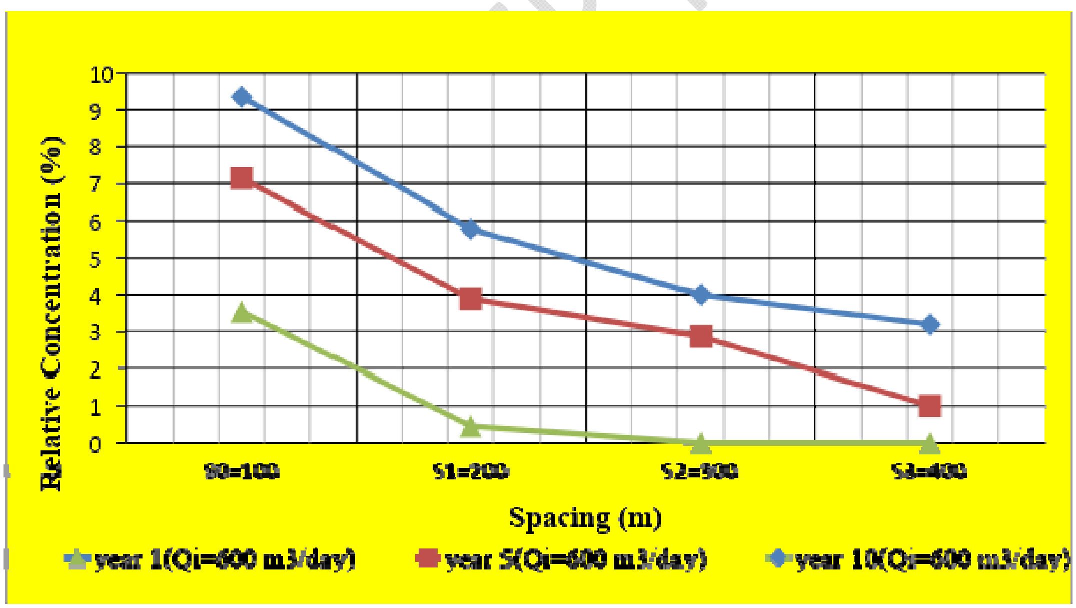

Fig. 6. Design chart for Q_i=600 m^3/day after 1, 5, 10 years of simulation

Fig. 7 represents the salt concentration distributions (shape of the salty plume) that develops around the injection well for a rate of injection equals 600 m^3/day at spacing equals 100 m after 10 years of simulation. It also shows that the salt plume migrates downward due to the high density of the injected brine into the aquifer.

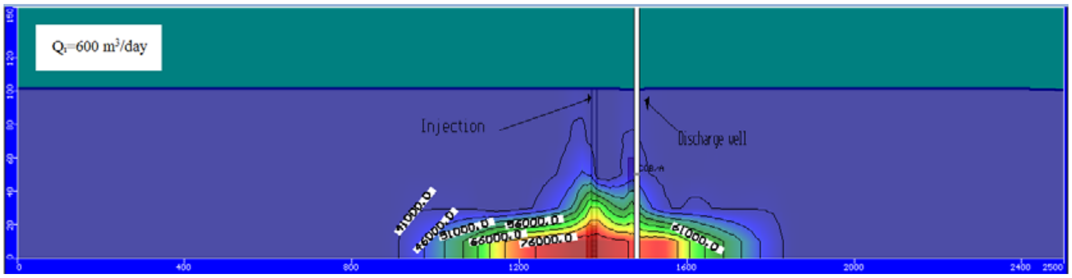

Fig. 7. Salt concentration distributions along x–z vertical plane after 10 years of simulation for injection rates 600 m^3/day at S=100 m

CONCLUSIONS

From this study we can conclude that:

1. There was an agreement between the results of the Visual MODFLOW and that of the laboratory experiment, where the correlation coefficient obtained from the model for the COB3, COB4 and COB5 were 0.991, 0.995 and 0.981 respectively. While for HOB1 and HOB2 were 0.901 and 0.835 respectively.
2. The relative salt concentration of groundwater is inversely proportional to the spacing between the injection and discharge wells.
3. The salt plume migrates downward due to the high density of the injected brine into the aquifer.
4. The Visual MODFLOW can assist engineers and researchers in simulating and predicting the impact of brine disposal on the groundwater salinity.

Competing interests: no competing interests exist

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