<u>Original Research Article</u> Validating Visual Modflow Numerical Model To Predict Future

3

1

2

Impact Of Brine Disposal On Groundwater

4

5 Abstract

6 The aim of this research is to simulate the groundwater extraction and brine disposal. The Visual 7 MODFLOW numerical model was used to predict the salt concentration emigration over time in a 8 groundwater aquifer. The main objective of this study is to verify and calibrate the Visual modflow 9 software for predicting the impact of brine disposal on the groundwater salinity.

10 Keywords: Brine disposal; Desalination; Groundwater; Injection well; Visual MODFLOW

11 INTRODUCTION

12 Desalination is one of the non-conventional water resources where fresh water is produced from 13 treatment of salt water. However, the negative impact of desalination process is the brine disposal 14 which is a real environmental problem that should be considered and studied before constructing a 15 desalination plant. The brine resulted from the desalination process is usually injected into a saline 16 aquifer or discharged into the sea. The practice of disposing the rejected brine into the sea is common 17 for plants located in coastal areas [1]. The problem of disposing the rejected brine into the sea may 18 change seawater salinity leading to injuring plants and animals in the marine sanctuary [3, 5, 6]. In the 19 case of disposing the rejected brine into the ground, it is necessary to design a disposal system in a way 20 that respects the environment. Nowadays, many mathematical models have been developed to 21 simulate groundwater flow.

In this research, the laboratory experiment of [4] is used to calibrate the Visual MODFLOW (VMOD).
 Then four scenarios were proposed, designed and simulated to study the process of groundwater
 extraction and rejected brine injection into a virtual aquifer using Visual modflow. The main objective of

this study is to calibrate and validate the Visual modflow software for predicting the impact of brinedisposal on the groundwater salinity.

27 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 that developed by [2] as shown in Eq. (1)

$$35 \qquad \frac{1}{\partial x} \left(\rho K_{fx} \left[\frac{\partial h_f}{\partial x} \right] \right) + \frac{\partial}{\partial y} \left(\rho K_{fy} \left[\frac{\partial h_f}{\partial y} \right] \right) + \frac{\partial}{\partial z} \left(\rho K_{fz} \left[\frac{\partial h_f}{\partial z} + \left(\frac{\rho - \rho_f}{\rho_f} \right) \right] \right) = \rho s_f \frac{\partial h_f}{\partial t} + \theta \frac{\partial \rho}{\partial c} \frac{\partial c}{\partial t} - \underline{\rho} q_s \tag{1}$$

36 Where ρ is the fluid density, K_{fx} , K_{fy} and K_{fz} are freshwater hydraulic conductivity in the x, y and z 37 direction, h_f is the equivalent fresh water head, ρ_f is the density of freshwater, S_f is the fresh water 38 specific storage, θ is the porosity, C is the concentration of solute mass per unit volume of fluid, q_s is the 39 volumetric flow rate of sources or sinks per unit volume of aquifer and t is time. The governing equation 40 for solute-transport is given by Eq. (2):

41
$$\frac{\partial(\theta C)}{\partial t} = \nabla(\theta D. \nabla C) - \nabla(qC) \pm q_s C_s$$
 (2)

42 Where:

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

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

45 Visual modflow calibration

46 VMOD model in the current research was calibrated with the experimental results conducted by [4] at

47 Hydraulic Laboratory of Cairo University, Giza, Egypt. The experiment setup was a rectangular seepage

48 tank with dimension of 1.42 m long, 0.1 m wide and 0.6 m high was used in the experimental work. An

- 49 injection well of 10 cm width was inserted on the left side of the seepage tank with a screen of 10 cm
- 50 width that located at 0.15 m from the base of the tank. While, a constant head boundary of 24.5 cm

- 51 was maintained on the right side of the tank. A constant head reservoir containing brine water of 39,400
- 52 ppm concentration is used to feed the injection well at a rate of $0.144 \text{ m}^3/\text{day}$.

53 Models domain

- 54 It consists of one row, 29 columns and five layers. Dimensions of cells in column 1 are 0.02m * 0.05m
- and cells in layer 1 are 0.05m * 0.2m. The rest of the cells are 0.05 by 0.05m.

56 Initial and boundary conditions

- 57 Initial concentrations of model domain are set to be 800 mg/l and initial fresh water heads are all set to
- 58 be 0.245 m. Brine is applied in column one and layer two through a well with injection rate 0.144
- 59 m³/day and of concentration equal to 39400 mg/l. A constant fresh water head boundary of 0.245 m
- 60 and a constant concentration equal to 800 mg/l are specified at column 29 and layer one.

61 Model parameters

- 62 The parameters used in this model are hydraulic conductivity, specific yield, porosity and coefficient of
- 63 effective molecular diffusion. The assigned values for these parameters were set to be 83 m/day, 0.27,
- 64 0.3 and $8.53*10^{-8}$ m²/min respectively.

65 **Observation Points**

- 66 Several observation points were constructed within the model domain as described in Table 1. The
- 67 records obtained from the head and concentration observation points are required during the
- 68 calibration process of the Visual MODFLOW model.

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

69 Table 1. Observation points locations

70 Time steps were set to be 24 steps to represent both head and concentration values for six hours model71 run.

72 Results of calibration

- 73 The outputs of the model are illustrated in Fig. 1 and Fig. 2. A comparison between the results obtained
- 74 from the VMOD and the laboratory experiment of [4] for the concentration observation points COB3,
- 75 COB4 and COB5 is shown in Fig. 1.

The correlation coefficient obtained from the model for these observation points were equal to 0.991, 0.995 and 0.981 respectively. While, Fig. 2 shows a comparison between the results obtained from the VMOD and the laboratory experiment of [4] for the head observation points HOB1 and HOB2.The correlation coefficient obtained from the model for HOB1 equal to 0.901and for HOB2 equal to 0.835.



80

81 Fig.1. Comparison between results of Visual MODFLOW and laboratory experiment of [4] for COB3,

COB4 and COB5

82



83

84 Fig. 2. Comparison between results of Visual MODFLOW and laboratory experiment of [4] for HOB1 and

85

HOB2

86 Visual MODFLOW APPLICATIONS

87 It is important to design a discharge system for brine disposal that respects the environment and predict its 88 effect on groundwater quality. Visual MODFLOW was used to detect the impact of brine disposal on the 89 groundwater salinity by simulating four scenarios on the virtual aquifer as discussed in the following 90 section.

91 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. 3. 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 m³/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.



99

Fig. 3. Virtual coastal area layout

- 100 Where:
- 101 Q_{inj} : is the rate of the injection well,
- 102 Q_d : is the rate of the discharge well
- 103 *C*_{inj} : is the concentration of the injection well,
- 104 S : is the spacing between the injection and the discharge wells,
- 105 C_i : is the initial concentration of the aquifer.

106 Visual Modflow simulation

107 Visual modflow was used to simulate the density-dependent flow and mass transport of the virtual 108 coastal area. The model domain consists of 75 rows, 125 columns and five layers. Cells of layer 2, 3, 4 109 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 110 in the horizontal, and 70 m in the vertical. A general head boundary condition (GHB) was assigned along 111 the outside edged of the model domain (column 1, row 1 and row 52) with conductance equal to 16 112 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.4. Ten time steps were used to represent both head and concentration values for ten years model run.



126 into the aquifer for different cases, four runs have been conducted as shown in Table 2.

127 Table 2. Simulated scenarios used in VMOD application

	Initial conc. of	Injection Conc	0	0	ç	κ*		
Scenarios	aquifer	injection conc.		\mathbf{Q}_i	5	K _X	d`∕d	К
	(mg/l)	(mg/l)	(m³/day)	(m³/day)	(m)	(m/day)		
1	40000	80000	1200	600	100	33	0.6	3
2	40000	80000	1200	600	200	33	0.6	3
3	40000	80000	1200	600	300	33	0.6	3
4	40000	80000	1200	600	400	33	0.6	3

128 ^{*} is the hydraulic conductivity of the aquifer.

129 Application Results and discussions

130 The results of the simulated scenarios are shown in Fig.5 and Fig. 6.

131 Fig.5 is the design chart that has been developed by three design parameters, relative salt concentration

132 (RSC), wells spacing (S), and simulation period (T). The Relative Salt Concentration at the discharge well

133 (*RSC*) is given by Eq. (3):

134
$$RSC = \left(\frac{C_P - C_i}{C_i}\right) * 100 \tag{3}$$

135 Where: C_P is the predicted concentration from VMOD, C_i is the initial concentration and *RSC* is the 136 relative salt concentration.

Fig. 5 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.



142

Fig. 5. Design chart for Q_i=600 m³/day after 1, 5, 10 years of simulation

Fig. 6 represents the salt concentration distributions (shape of the salty plume) that develops around the injection well for a rate of injection equals 600 m³/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. 6. Salt concentration distributions along x–z vertical plane after 10 years of simulation for

149

injection rates 600 m³/day at S=100 m

150 CONCLUSIONS

- 151 From this study we can conclude that:
- 152 1. There was a great agreement between the results of the Visual modflow and that of the
- 153 laboratory experiment, where the correlation coefficient obtained from the model for the
- 154 COB3, COB4 and COB5 were 0.991, 0.995 and 0.981 respectively. While for HOB1 and HOB2
- 155 were 0.901 and 0.835 respectivily.
- 156 2. Visual modflow model can be used as a useful tool for groundwater flow simulation.
- The Visual modflow can assist engineers and researchers in simulating and predicting the future
 impact of brine disposal on the groundwater salinity.
- 4. The relative salt concentration of groundwater is inversely proportional to the spacingbetween the injection and discharge wells.
- 161 5. The salt plume migrates downward due to the high density of the injected brine into theaquifer.
- 163 **Competing interests:** no competing interests exist

164 **REFERENCES**

- El-Naas M H, Al-Marzouqi A H, Chaalal O. A combined approach for the management of
 desalination reject brine and capture of CO2. Desalination. 2010;251:70–74.
 https://doi.org/10.1016/j.desal.2009.09.141
- Guo W, Langevin C D. User's guide to SEAWAT: a computer program for simulation of three dimensional variable-density ground-water flow. USGS Techniques of Water Resources
 Investigations chap A7. 2002.
- Mansour S, Arafat H A, Hasan S W. Brine Management in Desalination Plants. In Desalination
 Sustainability. Elsevier. 2017;207–236. https://doi.org/10.1016/B978-0-12-809791-5.00005-5
- Nassar M K K, El-Damak R M, Ghanem A H M. Impact of desalination plants brine injection wells
 on coastal aquifers. In Environmental Geology. 2008;54:445–454.
 https://doi.org/10.1007/s00254-007-0849-9

176 5. Petersen K L, Frank H, Paytan A, Bar-Zeev E. Impacts of Seawater Desalination on Coastal 177 Environments. In Sustainable Desalination Handbook: Plant Selection, Design and https://doi.org/10.1016/B978-0-12-809240-178 Implementation. Elsevier. 2018; 437-463. 179 8.00011-3 180 6. Tularam G A, Ilahee M. Environmental concerns of desalinating seawater using reverse 181 osmosis. Journal of Environmental Monitoring. 2007;9:805-813. https://doi.org/10.1039/b708455m 182 183 184