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Using simulation-optimization model in water resource management with consideration of environmental issues

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Abstract

Fast progress of countries has led to the expansion of industrial units. If this expansion be done without considering all aspects, especially environmental considerations, it may have some benefits in the short-term, but it causes sometimes heavy damages and sometimes irreparable damages in the long-term. So, a management system should monitor by using scientific instruments and methods in locating, designing, and exploiting these units. Modeling is a powerful tool that really helps in making decisions by simulating future conditions. Also, in a case that several parameters are involved in decision making, the best values of these parameters could be determined by using optimization technique and then the changes could be seen by using created model. In this paper, a management system is developed using MODFLOW and MT3DMS numerical models and SCE optimization technique for determining qualitative and quantitative conditions of wastewater disposal with the aim of clearing contamination in an assumed contaminated aquifer. Finally, considering the intended management goals, several different approaches were assessed.

Keywords: Simulation, Optimization, SCE, MODFLOW, MT3DMS

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Introduction

Environment is a great benefit to the human beings in all aspects. From soil, water to the air, it always provides a great opportunity to progress and develop human's life [1, 2]. It is a reliable source of energies such as geothermal, solar, wind etc. and always is in service of development of societies [3, 4, 5, 6]. However, fast progress of countries has led to the expansion of industrial units. If this expansion be done without considering all aspects, especially environmental considerations, it may have some benefits in the short-term, but it causes sometimes heavy damages and sometimes irreparable damages in the long-term [6, 7, 8]. Among these damages, we can mention the risks of wastewater disposal regardless of environmental conditions. So, when locating industrial units, attention should be paid to the amount of wastewater which is produced, groundwater conditions and the characteristics of the area. Also, if it's necessary, some changes should be applied during exploitation period, in order to reach intended management goals [9, 10]. So, a management system should monitor by using scientific instruments and methods in locating, designing, and exploiting these units [11]. In order to see qualitative and quantitative changes, numerical models for simulating underground water status can be used, recently many researchers are modeling the qualitative and quantitative changes with different approaches [12, 13, 14, 15]. Two of the most used and most accepted models are MODFLOW and MT3DMS which are used for simulating the changes in the level of underground water and for qualitative simulating of underground water, respectively [16]. These two models are developed and reported by U.S. Geological center and US Department of Defense, respectively. Considering the wide range of parameters affecting groundwater conditions and the existence of nonlinear relations, and in order to avoid waste of existing resources and capital, it is necessary to carefully determine the conditions for carrying out operations and to utilize scientific tools and methods as much as possible. Optimization methods are among these tools, which can be useful in selecting the correct parameters in order to achieve the most efficiency [17]. For example, Lara et al. used optimization methods in order to investigate the possibility of clearing a contaminated aquifer [18]. SCE is among meta-heuristic searching methods which is really effective in calibrating hydrological models and it has a high efficiency. In recent years, this algorithm is used by many researchers and it has been tested on different hydrological models [19, 20, 21, 22]. In this paper, a management system is developed using MODFLOW and MT3DMS numerical models and SCE optimization technique for determining qualitative and quantitative conditions of wastewater disposal with the aim of clearing contamination in an assumed contaminated aquifer. Finally, considering the intended management goals, several different approaches were assessed.

Methods and Materials:

By using continuity equation and by assuming a constant density for water, the three dimensional equation which rules over the flow, can be provided as follows:

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

In which x, y, and z are vectors of location, k_{xx}, k_{yy}, and k_{zz} are electrical conductivity in the x, y, and z direction, respectively (L/T), h is the hydraulic load (L), W is the amount of water removed or added by an external agent (L^3/T), Ss is the special storage (1/L), and t is the time (T).

Also, this subject that how is the three-dimensional movement of the contaminant inside the porous medium can be expressed by using the partial differential equation below:

$$\frac{\partial}{\partial x}(D_{xx}\frac{\partial c}{\partial x})+\frac{\partial}{\partial y}(D_{yy}\frac{\partial c}{\partial y})+\frac{\partial}{\partial z}(D_{zz}\frac{\partial c}{\partial z})-\left[\frac{\partial}{\partial x}(V_x c)+\frac{\partial}{\partial y}(V_y c)+\frac{\partial}{\partial z}(V_z c)\right]+W\frac{C_s}{\theta}+\sum_{k=1}^{N}R_k=R\frac{\partial c}{\partial t} \quad (2)$$

In which x, y, and z are vectors of location, D_{xx}, D_{yy}, and D_{zz} are hydrodynamic propagation factors in the x, y, and z direction (L^2/T), c is the contaminant concentration (M/L^3), V_x, V_y, and V_z are leakage speeds in x, y, and z direction, respectively (L/T), c_s is the concentration of production or removal of contamination (M/L^3), θ is the porosity, $\sum_{k=1}^{N} R(k)$ is the sum of chemical reaction terms, R is the delay factor, and t is the time (T). Transmission equations are related to the flow equations using the following equations:

$$V_x=-\frac{K_{xx}}{\theta}\frac{\partial h}{\partial x} \quad (3)$$

$$V_y=-\frac{K_{yy}}{\theta}\frac{\partial h}{\partial y} \quad (4)$$

$$V_z=-\frac{K_{zz}}{\theta}\frac{\partial h}{\partial z} \quad (5)$$

The evolutionary algorithm of mixed complexes (SCE) [19] is an evolutionary optimization method and its goal is to solve continuous optimization problems. The aim of designing this method is to search global minimum points in problems which have several local minimum points, like calibrating non-linear hydraulic simulation models. SCE is a meta-heuristic algorithm which is built based on four main concepts:

- Combining definitive and probabilistic methods
- A complex systematic evolution of points around the sample space
- Competitive evolution within each complex
- Mixing and sharing points among complexes

The steps of SCE algorithm are as follows:

First step: the number of complexes ($p\geq1$) and the number of points inside each complex ($m\geq n+1$) will be chosen, so the size of the sample (s) is equal to s=pm.

Second step: a sample population with s points ($x_1,\ldots,x_s$) are chosen from the possible space. Then the amount of f_i function is calculated for each point (x_i). Then the population of points will be ordered in an order in which the amount of matching is increasing. Then the ordered points will be stored in array $B=\{x_i, f_i, i=1,\ldots,s\}$, so that i=1 is the represent of minimum amount of function.

Third step: B will be divided into p complexes ($A^1,\ldots,A^p$) which each one has m points, so that

$$A^k = \left\{ x_j^k, f_j^k \middle| x_j^k = x_{k+p(j-1)}, f_j^k = f_{k+p(j-1)} \right\} j = 1,\ldots,m \tag{6}$$

Fourth step: each complex (A^k, k=1,…,p) will be evolved according to CCE algorithm [23].

Fifth step: complexes will be mixed. After the complexes evolved several times (which is specified), $A^1,\ldots,A^p$ are pasted in B, so that $B=\{A^k, k=1,\ldots,p\}$. Again, B will be ordered in an order in which the amount of function is increasing.

Sixth step: if the user-specified convergence factor is satisfied, the algorithm ends, otherwise the process returns to step 2. The algorithm of SCE method can be seen in figure1.

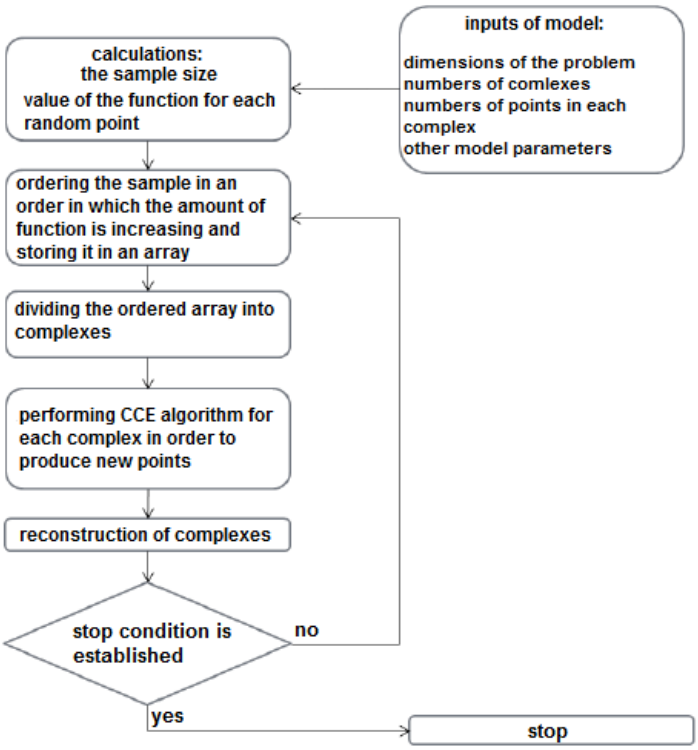


Figure1- flowchart of SCE algorithm

In the case of using figures and tables, necessarily, they should be referred in the text before representing them. Reference in the text will be like referring to the figure with a number (figure1). The numbering of the figures in the entire text of the article is continuous and it should not be individually numbered for each section. The figures and tables should be placed in the middle of the page and at a constant distance from the left and right margins. Note that the title of the figure should be placed below it and the title of the table should be placed on top of it.

In order to use the numerical model, first, we must attempt to network the studied area. The network of numerical model has 100 rows and 100 columns (figure2) and generally it encompasses a site with a length and a width of 5000 m and an area of 25000000 m^2 (2500 hectares). So, the dimensions of each cell is 50m*50m and the area of it is 2500 m^2. The boundary conditions include the boundaries of a fixed head of 275 meters in the north and 114.5 meters in the south, along with boundaries without any flows on the right and left of the range. The aquifer consists of a layer and it's of an open type. Other information of model is mentioned in table 1. In the north part of the range, 3 industrial units have disposed their wastewater in a non-standard way for one year, which has contaminated the aquifer. After standardization and removing the intended contaminants from the wastewater, industrial units have started to dispose their wastewater integrally in a range with an area of 10000 m^2 (100m*100m). There are 5 operation wells in this area which are exploiting the aquifer with a rate of flow of 500 cms. In order to investigate the changes in the level of water, there are also 4 observation wells in this range.

Table 1- Groundwater Model Parameters

Hydraulic conductivity	1. $1.389*10^{-4}$ m/s
Porosity	2. 0.35
Longitudinal propagation coefficient	3. 15 m
Propagation ratio	4. 0.15
Simulation time	5. 10 years

The intended goal is to maximize the disposal of wastewater by changing the entry rate in 4 cells of disposal pond and removal rate in 5 removal wells, in addition to try to minimize the changes in the level of water and the entry of contaminants into the exploitation wells. Consequently, the constraints of the problem are:

- The level of water in observation wells should be close to the intended amounts as much as possible.
- Concentration of contamination in removal wells should be reduced as much as possible.

The mathematical expression of the optimization model is as follows:

$$Maximize\left\{\sum_{r=1}^{N_b} A_r R_r\right\} - \left\{\sum_{w=1}^{N_w} Q_w\right\} \tag{7}$$

And also the constraints of the problem are:

$$h^j_{min} \le h_j \le h^j_{max}; j=1,\ldots,O_w \tag{8}$$

$$Q_{min} \le Q \le Q_{max} \tag{9}$$

$$R_{min} \le R \le R_{max} \tag{10}$$

$$D \le \sum_{w=1}^{N_w} Q_w \le Q^T \tag{11}$$

In which A_r is the area of wastewater disposal pool r, N_b is the number of all pools, R_r is the feed rate in pool r, R_{min} and R_{max} are upper and lower limits that are determined by physical and operational limitations, Q_w is the rate of removal from well w, N_w is the number of all removal wells, h_j is the simulated water level at observation point j, h^*_j is the intended water level at point j, h^j_{min} and h^j_{max} are minimum and maximum permitted range of simulated water level at point j, O_w is the number of all the observation wells, D is the amount of water demand that should be provided from removal wells, Q^T is the upper limit of total removal from wells which is allowed. Since SCE model is an unbound model, in the event of exceeding the constraints, amounts are considered as fines in the objective function. As a result, the objective function is as follows:

$$Minimize - \left\{\sum_{r=1}^{N_b} A_r R_r\right\} + \left\{\sum_{w=1}^{N_w} Q_w\right\} + P^1 + P^2. \tag{12}$$

$$P^1 = W_{p1} \left|h_j - h_j^*\right| \tag{13}$$

$$P^2 = W_{p2} C_W \tag{14}$$

That P^1 is the amount of fines for unauthorized changes of the simulated water surface relative to the target value (the amount of observed level at point) and P^2 is the amount of fines for the amount of contamination which enters operation wells. c_w is the contamination concentration in removal wells.

Results and Discussion

In order to maximize the use of operation wells, the problem conditions were determined in such a way to maximize the amount of wastewater disposal by considering the greatest reduction in the amount of contamination which entered into wells and the least change in groundwater level at the points (observation wells). Allowed changes range of parameters is presented in Table 2.

Table 2- Allowed changes range of parameters of the problem

Q_{min}	500 cms
Q_{max}	1750 cms
R_{min}	0.5 m/d
R_{max}	1.2 m/d
D	2500 cms
Q^T	8750 cms
W_{p1}	10000
W_{p2}	100000

The optimal wastewater disposal rate was equal to a maximum value of 1/2 m/d. Also, the amount of difference of head in the observation wells as well as the optimal amount of removal from the wells are presented in Tables 3 and 4, respectively.

Table 3- difference of head in observatory wells in optimal mode

Name of well	Position (row, column)	Difference of head (m)
O1	(53,71)	0.157
O2	(69,20)	0.132
O3	(78,80)	0.004
O4	(93,47)	0.019

Table 4- optimum removal amount from operation wells

Name of well	Position (row, column)	Optimum removal amount (cms)
W1	(10,53)	511.47
W2	(47,57)	1726.05
W3	(61,80)	1730.96
W4	(25,88)	518.91
W5	(87,91)	736.79

In order to investigate different choices, the sum of difference of head in observation wells and the sum of maximum contamination concentration in operation wells, and also the amount of target function for different amounts of feeding and removal have been compared in table 5. It can be seen that in optimum state, the amount of target function is less than other states.

Table 5- Allowed changes range of parameters of the problem

Feeding (m/d)	500	1750	500	1750	Optimum
Removal (cms)	0.5	1.2	0.5	1.2	Optimum
Sum of removal (cms)	2500	8750	2500	8750	5224.18
Sum of difference of head (m)	0.357788	0.765808	0.858551	0.400894	0.311605
Sum of maximum of contamination concentration (mg/l)	0.921501	0.971101	0.867102	0.913202	0.874802
Amount of function	93228.0336	108518.2248	85795.7004	92079.1214	83820.4083

Also, if the concentration of 0.3 mg/l is considered as the maximum allowable concentration, it can be seen that in wells No. 2 and No. 3, the contamination concentration exceeds this value during a period of time. These amounts are presented in table 6 for well w2 and table 7 for well w3. Also, the amount of removal in this period of time and also removal relative increase relative to the state that the amount of removal from wells is equal to the minimum amount (500 cms) and no wastewater is also used for

feeding (by deducing the removal amount that can't be consumed because of contamination) for these two wells are presented in the mentioned tables.

Table 6- comparing qualitative and quantitative features of well w2 in different states

Feeding (m/d)	0	0.5	0.5	1.2	1.2	1.2
Removal (cms)	500	500	1750	500	1750	1726.05
Duration of forbidding consumption (d)	558	470	500	310	361	320
Contaminated removal amount (m^3)	279000	235000	875000	155000	631750	552336
Removal relative increase (%)	0	2.85	256.57	8.02	272.3	271.78

Table 7- comparing qualitative and quantitative features of well w3 in different states

Feeding (m/d)	0	0.5	0.5	1.2	1.2	1.2
Removal (cms)	500	500	1750	500	1750	1726.05
Duration of forbidding consumption (d)	459	343	450	0	281	237
Contaminated removal amount (m^3)	229500	171500	787500	0	491750	410237
Removal relative increase (%)	0	3.75	259.02	14.84	278.15	278.93

According to the above results, it can be concluded that simultaneously the highest amount of wastewater removal, the lowest change in environmental conditions (difference of head), and also the lowest amount of contamination in operation wells can be guaranteed. Also, regarding the future condition and based on the results of created model, each of the other states can also be chosen.

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