Investigating the Optimization-Simulation Problem of Groundwater Remediation Under Various Scenarios

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Abstract

The efficiency of groundwater remediation by the pump-and-treat (PAT) method is affected by several components. The most important of these components is the pumping wells' location. In this research, hybrid optimization-simulation models were developed to find the appropriate groundwater remediation strategy using the PAT method. The GA-FEM and NSGA-II-FEM models were used to solve two optimization problems for a real aquifer (Ghaen aquifer). These optimization problems were investigated from one objective problem and two objective problems in three scenarios. In solving the single-objective optimization problems, the objective was to determine the optimal location of three, five, and seven pumping wells with a rate of 600 m3/day to minimize the mean of carcinogenic human health risk. The results indicated that the GA-FEM model has a good efficiency with 356.2302×10^{-6}, 356.2253×10^{-6}, and 356.2226×10^{-6} for three scenarios, respectively. The results indicated that increasing the number of pumping wells between scenarios one and two, 0.0013% and scenarios one and three 0.0021% improves the amount of mean carcinogenic human health risk. In the two-objective problems, the second objective function was defined as minimizing the drawdown of the groundwater head. The results of the two-objective problems in three scenarios indicated that the NSGA-II algorithm had a good performance and the NSGA-II algorithm provided a well-distributed set of solutions along the Pareto-optimal front. Also, the results indicated that when there are 5 pumping wells, the minimum mean of carcinogenic human health risk is 3.56226 and by adding two more pumping wells, this amount reaches 3.56225, while the rate of groundwater drawdown increases by 20 meters. Therefore, increasing the number of pumping wells from one limit not only does not have a significant effect on reducing pollution but also causes an increased groundwater drawdown.

Keywords: Contaminant concentration, Drawdown of groundwater head, Finite element method, Genetic algorithms, Health risk assessment.

1. Introduction

The main sources of groundwater contamination can be from natural or human-made sources. Natural resources can include seawater intrusion, decomposition of natural minerals in the earth's crust, and landslides (Eldho at al., 2018). In recent decades, groundwater quality has been severely affected due to improper use and management of groundwater resources. The human-made sources are plenty ranging from domestic sources like leakages from septic tanks and sewers, improper disposal of industrial waste, widespread use of chemicals in agriculture such as fertilizers and pesticides and many other human activities (Freeze and Cherry. 1979). As mentioned, other sources of pollution include improper disposal of waste. When landfills are not well insulated, waste leachate that contains hazardous materials such as heavy metals can easily percolate into

groundwater and contaminate it (Eldho et al., 2018).

Groundwater contamination and reducing groundwater quality have made groundwater remediation and better management an urgent need. Over the past few decades, groundwater pollution has become a major problem in many parts of the world. In many parts of the world, available groundwater is unsuitable for drinking and even agriculture. Besides, groundwater remediation methods, are very expensive. Therefore, in choosing the remediation method, an appropriate approach should be taken so that the contamination is effectively removed and the proper result is finally achieved. Therefore, optimization is very important in groundwater remediation (Eldho et al., 2018). In the discussion of groundwater pollution, Darabi and Ghafouri, (2007) and Guneshwor et al. (2018) have identified sources of pollutants and some other researchers have studied various methods of groundwater remediation such as in situ phytoremediation Kumar et al. (2015) and Mategaonkar et al. (2018) or pump and treatment method (Wang et al., 2018). However, the design of an efficient remediation system is done for various purposes. Remediation methods generally have many influential components. For example, the pump and treatment method has important components such as the position of the pumping well, the rate of pumping, the remediation time, and the rate of groundwater drawdown during pumping.

Different methods are used to solve the optimization problem of groundwater remediation. Some researchers have used nonlinear programming methods (Gorelick et al., 1984) or meta-heuristic algorithms such as AMALGAM (Ouyang et al., 2017), probabilistic multi-objective genetic algorithm (PMOGA) (Singh et al. 2008), niched Pareto genetic algorithm (Erickson et al., 2002).

One of the most important goals of groundwater remediation is to reduce the contaminant concentration to the permissible level. The carcinogenic human health risk can be directly or indirectly related to the contaminant concentration (Yang et al., 2013). Many researchers have introduced the reduction of contaminant concentration and pumping cost, or in other words the number of

pumping wells and pumping rate (Alexander et al, 2018) and some others the location of pumping wells (Sbai, 2019) and groundwater remediation time as the objective function of their optimization problem (Mategaonkar et al., 2018). Besides, researchers have used various methods such as finite difference method (He et al., 2017) finite element method (Esfahani et al., 2018) and meshfree method (Boddula and Eldho, 2017) (Seyedpour et al., 2019) and MODFOLW software (Joswig et al., 2017) (Singh et al., 2011) to solve the optimization problem of groundwater remediation. Younes et al. (2022) present a robust upwind MFE scheme is proposed to avoid such unphysical oscillations. The new scheme is a combination of the upwind edge/face centered Finite Volume (FV) method with the hybrid formulation of the MFE method. The scheme ensures continuity of both advective and dispersive fluxes between adjacent elements and allows to maintain of the time derivative continuously, which permits the employment of high-order time integration methods via the Method of Lines (MOL).

To our best acknowledge, it can be explained that the simultaneous consideration of different objectives in groundwater remediation is very important. Besides, it is essential to use an efficient S/O model that can be applied to real-world problems. Therefore, the purpose of this study is to provide S/O model that can find the best pumping wells location for the PAT system. So those different objectives such as minimizing the carcinogenic human health risk and groundwater head drawdown are considered simultaneously. Due to the purpose of this study, The GA-FEM and NSGA-II-FEM are optimization-simulation models. In these models, we use the finite element method for simulation and GA and NSGA-II for optimization. In this study, the decision variable is different nodes in the aquifer domain. After choosing the nodes by population we simulate head and contaminant transport. Then we calculate the objective function value. This cycle continues until the end of the number of Iterations. We present GA-FEM and NSGA-II-FEM optimization-simulation model. Also, the S/O model can determine optimal different arrangements of

pumping wells at the aquifer domain. So that according to the importance of each objective in a specific real case study, the decision maker can choose one of those arrangements.

2. Materials and Methods
2.1. Case study

In this study, the aquifer located in the Ghaen basin is also investigated. Ghaen study area with an area of 929.1 km^2 is located between longitudes 58° $53'$ $39''$ to 59° $24'$ $40''$ east and 33° $32'$ $07''$ to 33° $51'$ $20''$ north. The aquifer is recharged from the west and south by 8.28 and 3.61 Mm^3/year, respectively. 0.5 Mm^3 of groundwater is discharged annually from the east side of the aquifer. There is a contaminant resource with absorptive well. Through this absorptive well, various contaminants seepage

to the ground. Two of these contaminants are chloride and nitrate-nitrogen. These pollutants have amounts higher than the standard of wastewater in Iran. Figure (1) shows the position of the contaminant source and recharge and discharge zones. Also, there are 134 pumping wells in the Ghaen aquifer. Due to the aquifer grid and distance between nodes (200 m), 17 number of pumping wells were placed in nearest nodes and their pumping rate were added together. Also in Table (1) the values of contaminants and their permissible limits are given. In order to using hydraulic information for aquifer modeling, at first, we create thiessen polygon for hydraulic conductivity by using ArcGIS software. Five-days' time step is chosen for both the groundwater flow and the contaminant transport model.
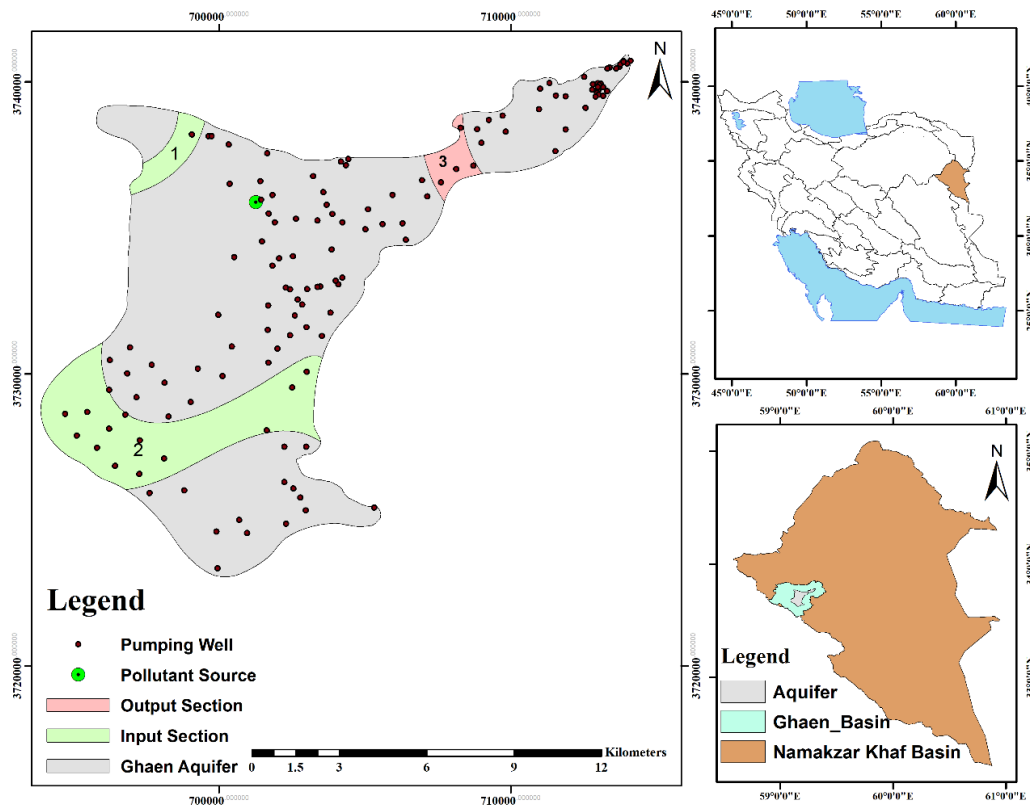

Fig. 1. Location map of the study area

Table 1. Contaminant values and standard values in Iran

Contaminant	Symbol	Unit	Value	Permissible limit
Sulfate	SO_4^{--}	mg/lit	452	400
Chloride	Cl^-	mg/lit	643.2	600
Nitrate-Nitrogen	NO_3-N	mg/lit	19.6	10

2.2. Objective functions

PAT system costs depend on the residual contaminant concentration at the end of the

remediation period. Two objective functions are considered in this case. These objective functions are (1) Minimizing the mean of

carcinogenic human health risk, (2) Minimizing the drawdown of the aquifer head. Therefore, the purpose of this study is to determine the optimal location of pumping wells so that objective functions are minimized. We consider three scenarios in one and two-objectives problems. In the first to third scenario, the number of wells is 3, 5 and 7 pumping wells, respectively, and the amount of pumping from each well is 600 m³/day. Also, the remediation time in all scenarios is considered 3 years. The objective functions are defined mathematically as follows:

$$Min \quad F_1 = \left(\sum_{k=1}^{K} ELCK_k \right) / K \tag{1}$$

$$Min \quad F_2 = \sum_{i=1}^{NNODE} \left(H_i^{old} - H_i^{new} \right) \tag{2}$$

where F_1 and F_2 are the objective functions 1 and 4, respectively.

In the first objective function minimizes the mean of carcinogenic human health risk where, K is number of monitoring wells and $ELCK_k$ is carcinogenic human health risk in k^{th} nodes.

In the second objective function minimizes the drawdown of the aquifer head where, H_i^{old} and H_i^{new} are aquifer head before and after installing pumping wells at i^{th} node, (m), respectively. NNODE is the total number of nodes in the aquifer domain. In addition, the constraint of the PAT optimization model are as follows:

$$c_k^{\left(q_j^{Ex} \right)} \leq c_{max} \quad k = 1, 2, ..., K \tag{3}$$

$$0 \leq q_j^{Ex} \leq q_{max}^{Ex} \quad j = 1, 2, ..., J \tag{4}$$

$$ELCK_k \leq ELCK_{max} \quad k = 1, 2, ..., K \tag{5}$$

$$ELCK_k = SF \times CDI_k \tag{6}$$

$$CDI_k = CW_k / 1000 \times IR \times EF \times ED / (AT \times BW) \tag{7}$$

where q_{max}^{Ex} is the maximum pumping rate from j^{th} pumping well (m³/hr). C_k contaminant concentration at k^{th} monitoring well (µg/L). Also, C_{max} is the maximum contaminant concentration (µg/L). ELCKmax is the maximum of carcinogenic human health risk. *SF* is a slope factor that is related to carcinogenic health risk, (kg day/mg); CDI_k is the daily intake of given contaminant at exposure location *k*, (mg/kg day); CW_k is the concentration of exposed contaminant at exposure location *k*, (µg/L); *IR* is the ingestion rate, (L/day); *EF* is exposure frequency, (day/year); *ED* is exposure duration, year; *AT* is average time, (day); and *BW* is body weight, (Kg) (Yang et al., 2018).

2.3. Governing equations
2.3.1. Groundwater flow modeling

The governing partial differential equations describing the steady-state flow in a two-dimensional inhomogeneous, anisotropic confined and unconfined aquifers are given as (Wang and Anderson, 1995):

$$\frac{\partial}{\partial x}\left(T_x \frac{\partial H}{\partial x} \right) + \frac{\partial}{\partial y}\left(T_y \frac{\partial H}{\partial y} \right) = R \tag{8}$$

$$\frac{\partial}{\partial x}\left(k_x H \frac{\partial H}{\partial x} \right) + \frac{\partial}{\partial y}\left(k_y H \frac{\partial H}{\partial y} \right) = R \tag{9}$$

Moreover, the governing partial differential equations describing the Transient flow in a two-dimensional inhomogeneous, anisotropic confined and unconfined aquifers are given as (Wang and Anderson, 1995):

$$\frac{\partial}{\partial x}\left(T_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y}\left(T_y \frac{\partial h}{\partial y} \right) = $$
$$S \frac{\partial h}{\partial t} + Q_w \delta(x - x_i)(y - y_i) - q \tag{10}$$

$$\frac{\partial}{\partial x}\left(K_x h \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y}\left(K_y h \frac{\partial h}{\partial y} \right) = $$
$$S_y \frac{\partial h}{\partial t} + Q_w \delta(x - x_i)(y - y_i) - q \tag{11}$$

where h(x,y,t) or H(x,y,t) is the piezometric head [L], $T_i(x,y)$ is anisotropic transmissivity [L²T⁻¹]; $K_i(x,y)$ is anisotropic hydraulic conductivity [LT⁻¹]; S(x,y) is storage coefficient, $S_y(x,y)$ is specific yield; Q_w is source or sink function; ($-Q_w$ = source and Q_w = sink) [LT⁻¹]; δ is Dirac delta function; x_i and y_i are the pumping or recharge well location; q(x,y,t) is vertical inflow rate [LT⁻¹]; x and y are horizontal space variables [L] and t is the time [T].

The seepage velocity necessary to the solution of the solute-transport model is computed using Darcy's law and can be written as: $V_i = -\frac{K_i}{\theta} \frac{\partial h}{\partial x_i}$, $i = x, y$ where $V_i(x,y)$ is seepage velocity in i-direction [LT⁻¹]; and θ is porosity [-] (Bear, 1988).

2.3.2. FEM to solve governing equations for groundwater flow

Using Galerkin's finite element method and two-dimensional element for approximation Eq (12), the first step is to define a trial solution.

$$\hat{h}(x,y,t) = \sum_{L=1}^{NP} h_L(t) N_L(x,y) \qquad (12)$$

where h_L is the unknown head, N_L is the known basis function at node L, and NP is the total number of nodes in the hypothetical aquifer domain. A set of simultaneous equations is obtained when residuals weighted by each of the basis function are forced to be zero and integrated over the entire domain Ω (Darabi and Ghafouri, 2007). Thus, Eq (12) can be written as:

$$\int\int_{\Omega} \left\lfloor \frac{\partial}{\partial x}\left(T_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_y \frac{\partial h}{\partial y}\right) - Q_w + q - S\frac{\partial h}{\partial t} \right\rfloor \qquad (13)$$
$$N_L(x,y)dxdy = 0$$

$$\sum_e \int \left(T_x^e \frac{\partial \hat{h}^e}{\partial x}\left\{\frac{\partial N_L^e}{\partial x}\right\} + T_y^e \frac{\partial \hat{h}^e}{\partial y}\left\{\frac{\partial N_L^e}{\partial y}\right\} \right) dxdy$$
$$+ \sum_e \int \left(S\frac{\partial \hat{h}^e}{\partial t} \right)\{N_L^e\}dxdy \qquad (14)$$
$$= \sum_e \int (Q_w)\{N_L^e\}dxdy - \sum_e \int (q)\{N_L^e\}dxdy$$

$$\text{where } \{N_L^e\} = \begin{Bmatrix} N_i \\ N_j \\ N_m \\ N_n \end{Bmatrix}.$$

For an element, Eq (14) can be written in matrix form as:

$$\left[G^e\right]\{h_I^e\} + \left[P^e\right]\left\{\frac{\partial h_I^e}{\partial t}\right\} = \{f^e\} \qquad (15)$$

where I = i, j, m, n are four nodes of rectangular elements and G, P, f are the element matrices known as conductance, storage matrices, and recharge vectors, respectively. Summation of elemental matrix Eq (15) for all the elements gives the global matrix as:

$$[G]\{h_I\} + [P]\left\{\frac{\partial h_I}{\partial t}\right\} = \{f\} \qquad (16)$$

Applying the implicit finite difference scheme for $\frac{\partial h_I}{\partial t}$, term in time domain for Eq (16) gives.

$$[G]\{h_I\}_{t+\Delta t} + [P]\left\{\frac{h_{t+\Delta t} - h_t}{\Delta t}\right\} = \{f\} \qquad (17)$$

The subscripts t and t + Δt represent the groundwater head values at earlier and present time steps. By rearranging the terms of Eq (17), the general form of the equation can be given as (Darabi and Ghafouri, 2007):

$$\left\lfloor [P] \right\rfloor + \omega\Delta t[G]\{h\}_{t+\Delta t} =$$
$$\left[\begin{array}{c} [P] - (1-\omega)\Delta t[G]\{h\}_t + \\ \Delta t(1-\omega)\{f\}_t + \omega\{f\}_{t+\Delta t} \end{array} \right] \qquad (18)$$

Where Δt = time step size, $\{h\}_t$ and $\{h\}_{t+\Delta t}$ are groundwater head vectors at the time t and t + Δt, respectively, x is Relaxation factor which depends on the type of finite difference scheme used. For fully explicit scheme $\omega = 0$; Crank–Nicolson scheme $\omega = 0.5$; fully implicit scheme $\omega = 1$.

2.3.3. Contaminant transport modeling

The governing differential equation is obtained based on the mass balance of any particular solute in a control volume of porous media. The final unsteady form of the equation, including adsorption and other chemical reactions, is written as follows (Darabi and Ghafouri, 2007):

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C}{\partial z}\right)$$
$$- v_x \frac{\partial C}{\partial x} - v_y \frac{\partial C}{\partial y} - v_z \frac{\partial C}{\partial z} + CHEM \qquad (19)$$

The seepage velocity required to the solute-transport model is calculated using Darcy's law and is written as: $V_i = -\frac{K_i}{\theta}\frac{\partial h}{\partial x_i}$, $i = x, y$; where $V_i(x,y)$ is the seepage velocity in i-direction [LT^{-1}]; and θ = porosity (Wang and Anderson, 1995).

In which C is the concentration of contamination at any given time and space, D the dispersion coefficient, and V is the seepage velocity. The first three terms at RHS show the dispersion phenomena while the second three terms represent the advection of contaminant. Also, CHEM consists of the following (Darabi and Ghafouri, 2007):

$$CHEM = -\frac{\rho_b}{n}\frac{\partial s}{\partial t} \qquad (20)$$

Which indicates the superficial forces of adsorption and ionization processes, and

$$CHEM = -\lambda\left(C + \frac{\rho_b}{n}s\right) \qquad (21)$$

In the above equations ρ_b is the bulk soil density (ML^{-3}), λ is constant decay coefficient (T^{-1}), s is the density of absorbed substance on soil grains or colloids, and *n* is the soil porosity. Substituting these terms into Eq (21) and simplifying them, results in the following equation (Bear, 2007):

$$
\begin{aligned}
\frac{\partial C}{\partial t} + \frac{\rho_b}{n} \frac{\partial s}{\partial t} \\
= \frac{\partial}{\partial x}\left(D_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial C}{\partial y}\right) + \\
\frac{\partial}{\partial z}\left(D_z \frac{\partial C}{\partial z}\right) - v_x \frac{\partial C}{\partial x} - v_y \frac{\partial C}{\partial y} \\
- v_z \frac{\partial C}{\partial z} - \lambda\left(C + \frac{\rho_b}{n} s\right)
\end{aligned}
\tag{22}
$$

Assuming s = $k_d \times$ C, where k_d is a distribution coefficient, applying the chain rule to the derivative of s and re-ordering the resulted relations, Eq (22) may be written as follows:

$$
\begin{aligned}
R \frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C}{\partial z}\right) \\
- v_x \frac{\partial C}{\partial x} - v_y \frac{\partial C}{\partial y} - v_z \frac{\partial C}{\partial z} - R\lambda C
\end{aligned}
\tag{23}
$$

Eq (19) is three dimensional governing equation of advection-dispersion of contaminants in groundwater resources where $R = 1 + \frac{\rho_b k_d}{n}$ is the retardation factor with ρ_b = media bulk density [ML^{-3}], and K_d = sorption coefficient [L^{3}M^{-1}]; C(x,y,t) is solute concentration [ML^{-3}]; D_x and D_y are components of dispersion coefficient tensor [L^{2}T^{-1}]; λ is the reaction rate constant [T^{-1}].

For transient flow and transport analysis, the following initial conditions are used:

$$
\begin{aligned}
h(x,y,0) = h_0(x,y); C(x,y,0) = f \\
x, y \in \Omega
\end{aligned}
\tag{24}
$$

The flow and transport equations should be solved with appropriate boundary conditions. The boundary conditions can be written as:

$$
\begin{aligned}
h(x,y,t) = h_1(x,y,t); C(x,y,t) = g_1 \\
x, y \in \Gamma_1
\end{aligned}
\tag{25}
$$

$T\frac{\partial h}{\partial n} = q_1(x,y,t)$ is for confined aquifer,

$Kh\frac{\partial h}{\partial x} = q_2(x,y,t)$ is for unconfined aquifer:

$$
\left(D_x \frac{\partial C}{\partial x}\right)n_x + \left(D_y \frac{\partial C}{\partial y}\right)n_y = g_2 \quad x, y \in \Gamma_2
\tag{26}
$$

where Ω is flow region; $\Gamma = \Gamma_1 \cup \Gamma_2$ is region boundary; $\frac{\partial}{\partial m}$ is normal derivative; $h_0(x,y)$ is initial head in the flow domain [L]; $h_1(x,y,t)$ is the known head value at the boundary section Γ_1 [L]; f is a given function in Ω, g_1 and g_2 are given functions along boundary sections Γ_1 and Γ_2; and $n_x n_y$ are the components of the unit outward normal vector to the boundary section Γ_2.

2.3.4. FEM to solve the governing equation for contaminant transport

The analytical solution of Eq. 17 is usually unavailable for aquifers having irregular geometries and/or boundary conditions. Hence an approximate numerical solution of the equation is often sought in most cases. The method of finite elements is one of the most frequently used methods for this purpose. This method is implemented whit a variety of element types and number of nodes. The elements join together and then, approximate solution of the sought unknown, i.e. the pollutant concentration (C$_L$), is computed at nodal points. For any other given point, the concentration value is approximated as (Darabi and Ghafouri, 2007):

$$
C(x,y,z,t) = \sum_{L=1}^{NNODE} C_L(t).N_L(x,y,z)
\tag{27}
$$

where $N_L(x,y,z)$ is an arbitrary approximating function, called shape function, of node L. Applying the finite element method to Eq. 23 leads to a set of simultaneous algebraic equations as:

$$
[A]\{C\}^{t+\Delta t} = [B]\{C\}^t + \{f\}
\tag{28}
$$

Where:

$$
[A] = [G] + [U] + [F] + \frac{1}{\Delta t}[P]
\tag{29}
$$

$$
[B] = \frac{1}{\Delta t}[P]
\tag{30}
$$

Δt is the length of time interval, the so-called time-step, $\{C\}^t$ is the vector of known concentrations at the beginning of any time step and $\{C\}^{t+\Delta t}$ is the vector of sought unknown concentrations at the end of the time step. [G], [U], [F], and [P] are square matrices in which the number of rows and columns is

equal to the number of nodal points in the computational grid. The elements of these matrices are computed as follows (Darabi and Ghafouri, 2007):

$$G_{(L,i)}^e = \int \int_e \left(\begin{array}{c} D_x \dfrac{\partial N_i^e}{\partial x} \dfrac{\partial N_L^e}{\partial x} \\[6pt] +D_y \dfrac{\partial N_i^e}{\partial y} \dfrac{\partial N_L^e}{\partial y} \\[6pt] +D_y \dfrac{\partial N_i^e}{\partial y} \dfrac{\partial N_L^e}{\partial y} \end{array} \right) dxdydz \qquad (31)$$

$$P_{(L,i)}^e = \iint_e R.N_i^e N_L^e dxdydz \qquad (32)$$

$$U_{(L,i)}^e = -\int \int_e \left(\begin{array}{c} V_x^e \dfrac{\partial N_i^e}{\partial x} N_L^e \\[6pt] +V_y^e \dfrac{\partial N_i^e}{\partial y} N_L^e \\[6pt] +V_z^e \dfrac{\partial N_i^e}{\partial z} N_L^e \end{array} \right) dxdydz \qquad (33)$$

$$F_{(L,i)}^e = -\iint_e R.\lambda.N_i^e N_L^e dxdydz \qquad (34)$$

{ f } is the load vector calculated using the following boundary integral:

$$\{f\} = \int_\Gamma \left(D_x \dfrac{\partial \hat{c}}{\partial x} n_x + D_y \dfrac{\partial \hat{c}}{\partial y} n_y + D_z \dfrac{\partial \hat{c}}{\partial z} n_z \right) N_L d\Gamma \qquad (35)$$

Where $\hat{c}$ denotes the given concentration values at boundary nodes, n_i are directional cosines and Γ is the domain boundary (Zeynali, 2022).

2.4. GA and NSGA-II algorithms

In the genetic algorithm (GA) and its multi-objective version (Non-Dominated Sorting Genetic Algorithm, NSGA-II), there are the crossover and mutation phases. In the single-objective version, population is sorted by the value of the objective function, and the selection of the best individual is based on the objective function value (Akbarpour et al., 2020). In the NSGA-II algorithm, the rank of each solution in the population is based on the non-dominated sorting and crowding distance. That is, members of the population on the first front are better than those on the second front. Members on the same front are ranked by crowding distance (Felfli et al., 2002).

2.5. Validation of FEM model

Before applying FEM model for the hypothetical and the real aquifer, the FEM model must be validated. For this purpose, our FEM model is compared with the analytical solution Kulkarni (2015) research (Kulkarni, 2015). In the Kulkarni's research, he assumed a hypothetical aquifer 3200m×2800m. Boundary conditions at the right and left sides of the aquifer boundary is considered no flow boundaries. Boundary conditions at the bottom and top sides of the aquifer boundary is considered to have constant value of 100m. The location of two pumping wells is (1400m, 1400m) and (1800m, 1400m) from the origin, as shown in Figure 2.
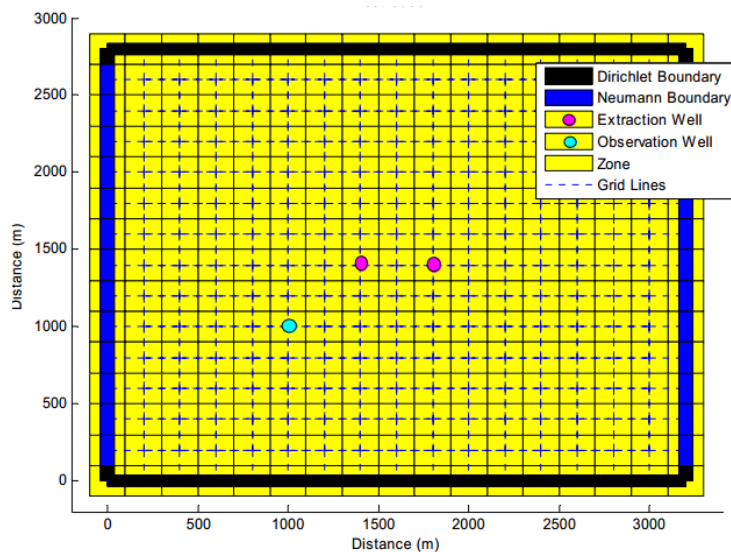

Fig. 2. Schematic of aquifer modeled for the validation of FEM model

The observation well is located at a (1000m, 1000m) from the origin and the water table

drawdown caused by pumping are observed at this well (Zeynali, 2022).

3. Results and Discussion

3.1. Validation

Pumping by two wells for 210 days cause the groundwater head drawdown, which was calculated using the FEM model. Analytical solution and FEM model are compared as shown in Figure 3. As can be seen from Figure 3, the drawdown value is computed as 0.4283 m by finite element method which are comparable with the drawdown of 0.4359 m by analytical solution. The most difference between the modeling results and the analytical solution was about 0.0440 m in the 81th days of the pumping period.

3.2. The results of the first scenario

In the first scenario, the optimization problem is investigated by considering three pumping wells with constant pumping rates (600 m^3/day). Also, the remediation time is 3 years. The present problem was investigated as one objective and two objectives.

3.2.1. Results of One-Objective problem

The optimization problem is finding of the three pumping wells in the aquifer domain to obtain the optimal values (close to optimal) for the first objective function. It should be noted that the first step in the pump and treat process is to remove the source of contaminants or prevent leakage of contamination, and then the pumping wells are installed for pumping contaminants.

The genetic algorithm ran five times with 10 population members and 20 iterations. The results of five runs of this algorithm, including the best, the worst, and average values of the objective function in five runs are given in Table (2). As can be seen in this table, the genetic algorithm with an average of 356.2302×10^{-6} has shown good performance. Also, the performance of GA for five runs is shown in Figure (4).

Also, the position of pumping wells and the concentration of Sulfate contaminant in the aquifer after 3 years of remediation are shown in Fig. 5.

Table 2. Statistical characteristics of the GA performance

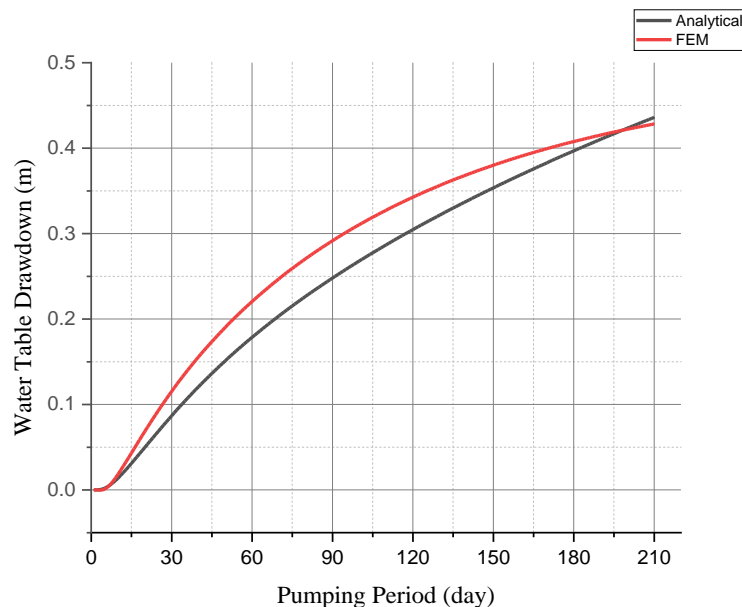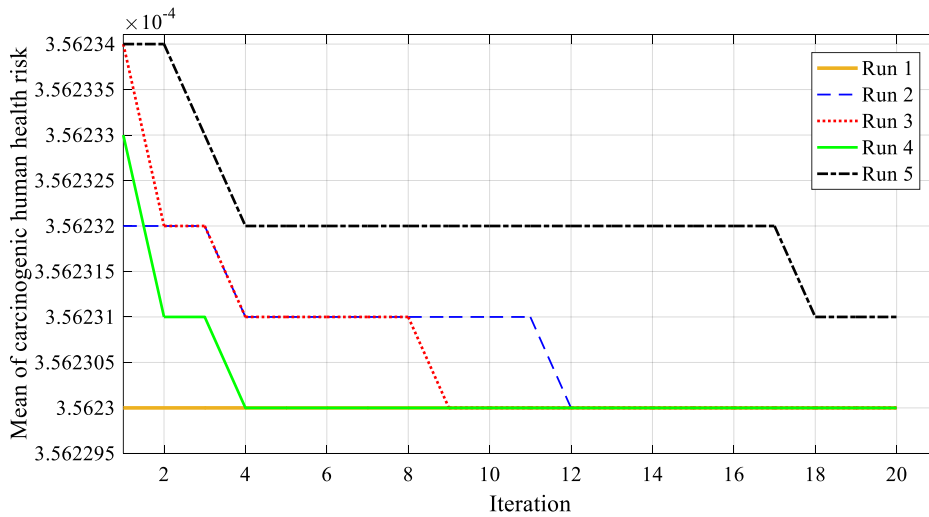| Algorithm	Best Value	Worst Value	Average values
GA	356.2300×10^{-6}	356.2307×10^{-6}	356.2302×10^{-6}

Fig. 3. Validation of FEM model
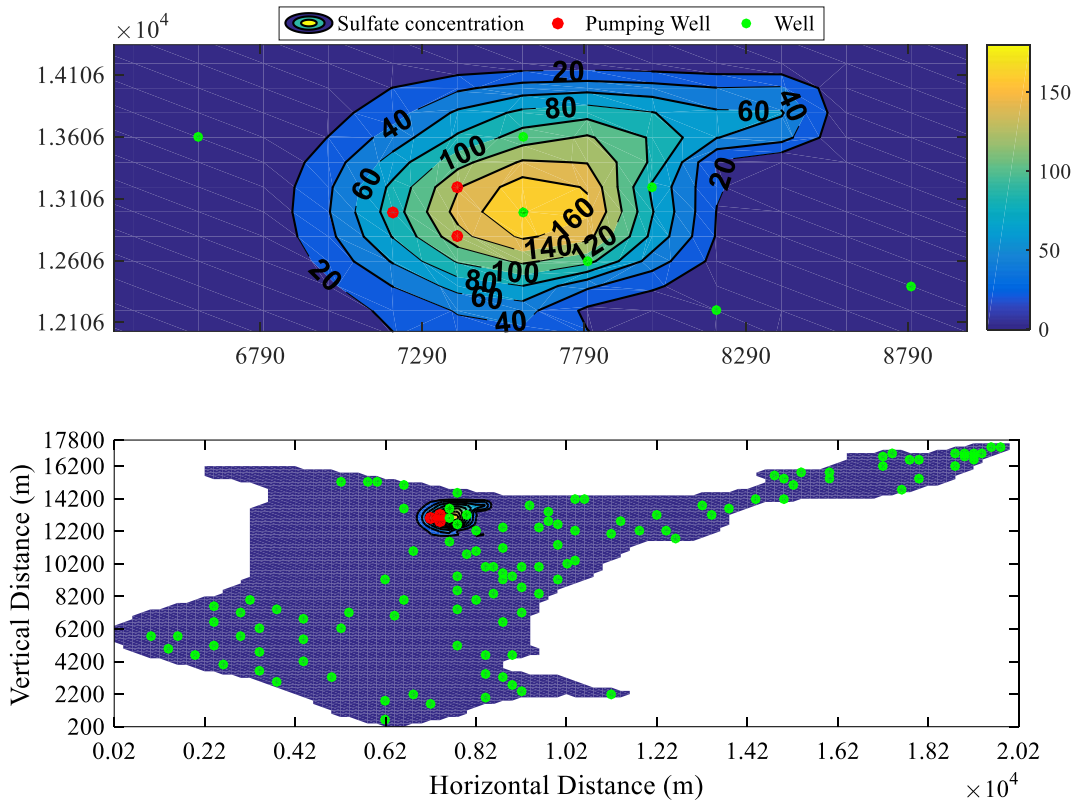
Fig. 4. The convergance trend of GA algorithm

Fig. 5. Sulfate concentration distribution in Aquifer (µg/Lit) and pumping well locations

3.2.2. Results of Two-Objective problem

In Two-Objective optimization problem, we find the best location of wells to find the minimum of contaminant concentrations and drawdown of the aquifer head. In NSGA-II algorithm, like single-objective version, 70% of the population could be parents, and the mutation rate was set to 90%. NSGA-II is run three times. The number of solutions in the Pareto-optimal front for run 1 to run 3 are 8, 8

and 9, respectively. The results of all runs shown in Fig. 6.

As it can be seen in this figure, NSGA-II algorithm find the solution with minimum of first objective function in run 3. Also, NSGA-II algorithm find the solution with minimum of second objective function in run 2. But, we can consider run 1 as the best performance of NSGA-II algorithm. Because this run of NSGA-II algorithm has a good coverage on

solution space. Also, run 1 could to find the minimum for two objective functions.

3.3. Results of second scenario

In second scenario, the optimization problem is investigated by considering five pumping wells with constant pumping rates (600 m³/day). Also, the remediation time is 3 years. The present problem was investigated as one-objective and two-objectives.

3.3.1. Results of One-Objective problem

The genetic algorithm run five times with 10 population members and 20 iterations. The results of five run of this algorithm, including the best, the worst and average values of the objective function in five run are given in Table (3). As can be seen in this table, the genetic algorithm with an average of 356.2253×10^{-6} has shown good performance. Also, the performance of GA for five run is shown in Fig. 7.

Also, the position of pumping wells and the concentration of Nitrate-Nitrogen contaminant in the aquifer after 3 years of remediation are shown in Fig. 8.

Table 3. Statistical characteristics of the GA performance

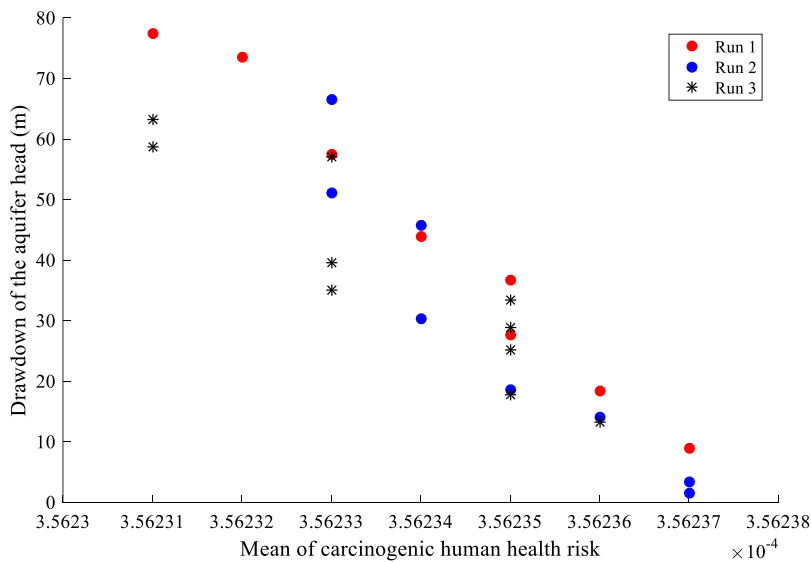| Algorithm	Best value	Worst value	Average values
GA	356.2253×10^{-6}	356.2268×10^{-6}	356.2261×10^{-6}

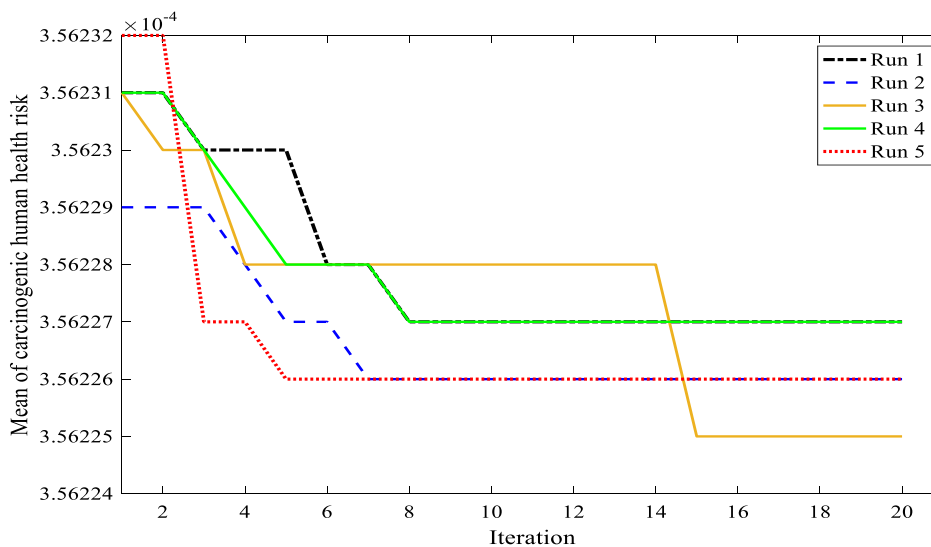**Fig. 6.** Pareto fronts in NSGA-II algorithm (Three Wells)
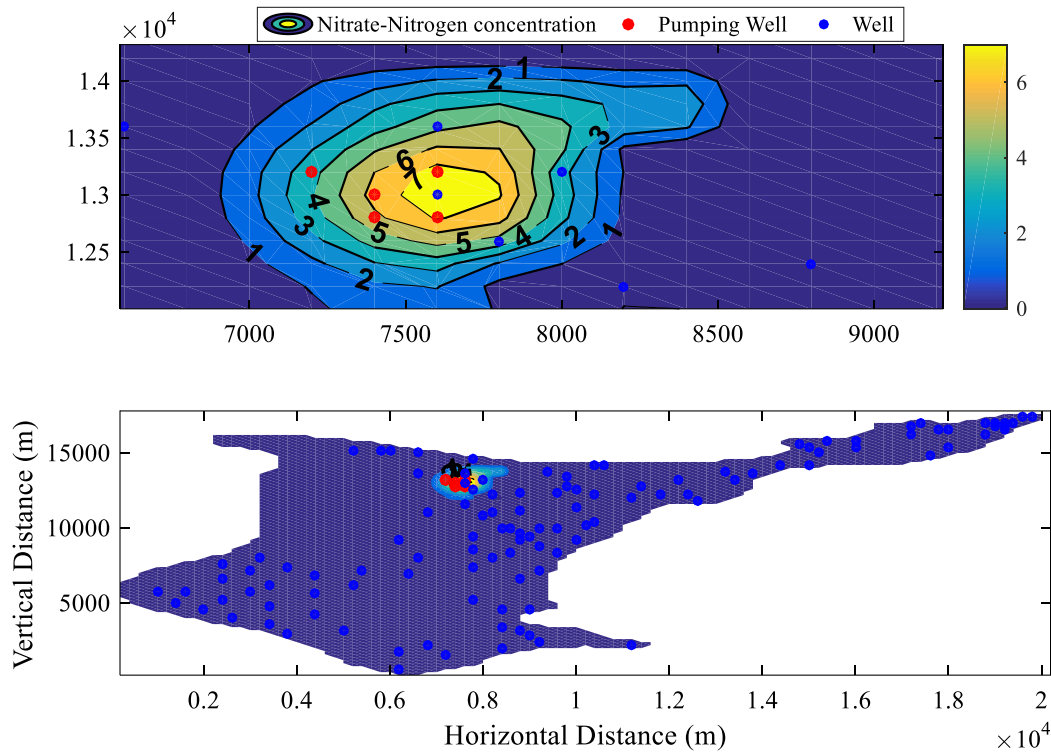

Fig. 7. The convergence trend of GA algorithm

Fig. 8. Nitrate-Nitrogen concentration distribution (*µg/Lit*) and pumping well locations

3.3.2. Results of Two-Objective problem

The results of all three runs for second scenario shown in Fig. 9. We can consider run 2 as the best performance of NSGA-II algorithm. Because this run of NSGA-II algorithm has a good coverage on solution space. Also, run 2 could to find the minimum for two objective functions.

3.4. Results of third scenario

In third scenario, the optimization problem is investigated by considering seven pumping wells with constant pumping rates (600 m^3/day). Also, the remediation time is 3 years. The present problem was investigated as one-objective and two-objectives.

3.4.1. Results of One-Objective problem

The genetic algorithm run five times with 10 population members and 20 iterations. The results of five run of this algorithm, including the best, the worst and average values of the objective function in five run are given in Table (4). As can be seen in this table, the

genetic algorithm with an average of 356.2226×10^{-6} has shown good performance. Also, the performance of GA for five run is shown in Fig. 10.

Also, the position of pumping wells and the concentration of Chloride contaminant in the aquifer after 3 years of remediation are shown in Fig. 11.

Table 4. Statistical characteristics of the GA performance

Algorithm	Best value	Worst value	Average values
GA	356.2226 ×10^{-6}	356.2247 ×10^{-6}	356.2236 ×10^{-6}

3.4.2. Results of Two-Objective problem

In two objective problems for third scenario, optimization-simulation model run three times. The Pareto front shown in Fig 12. It can be seen in this figure that run 2 and 3 are the best. Because provide a well-distributed set of solutions along the Pareto-optimal front. Also, it can be seen that number of solutions in this scenario are more than number of solutions in other scenarios.
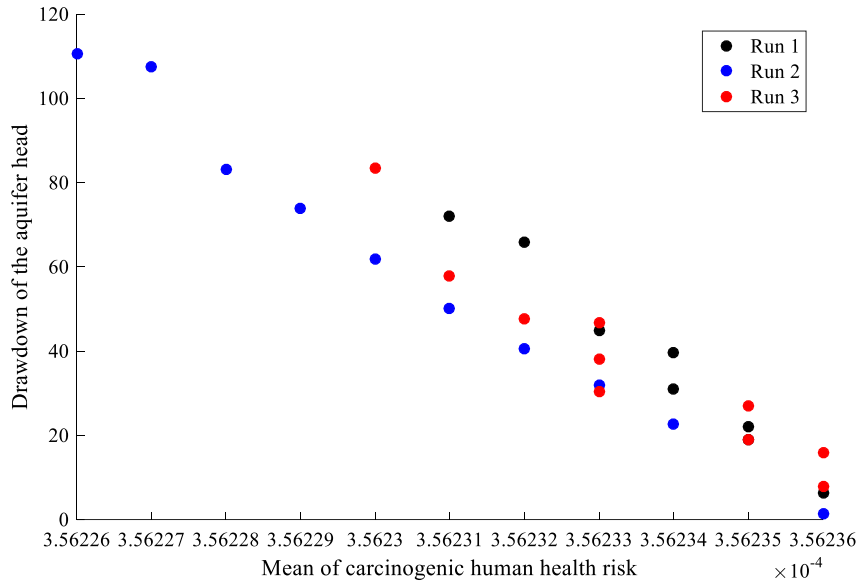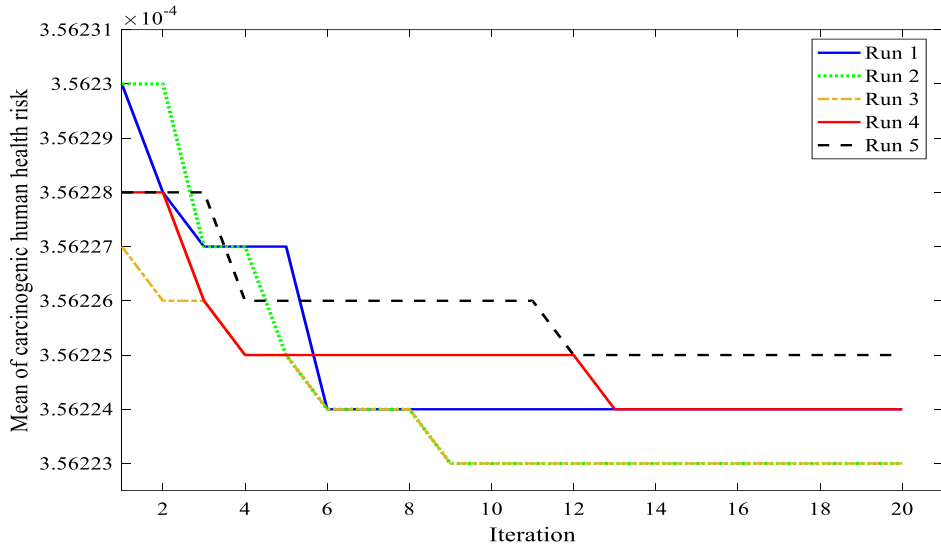
Fig. 9. Pareto fronts in NSGA-II algorithm (Five Wells)
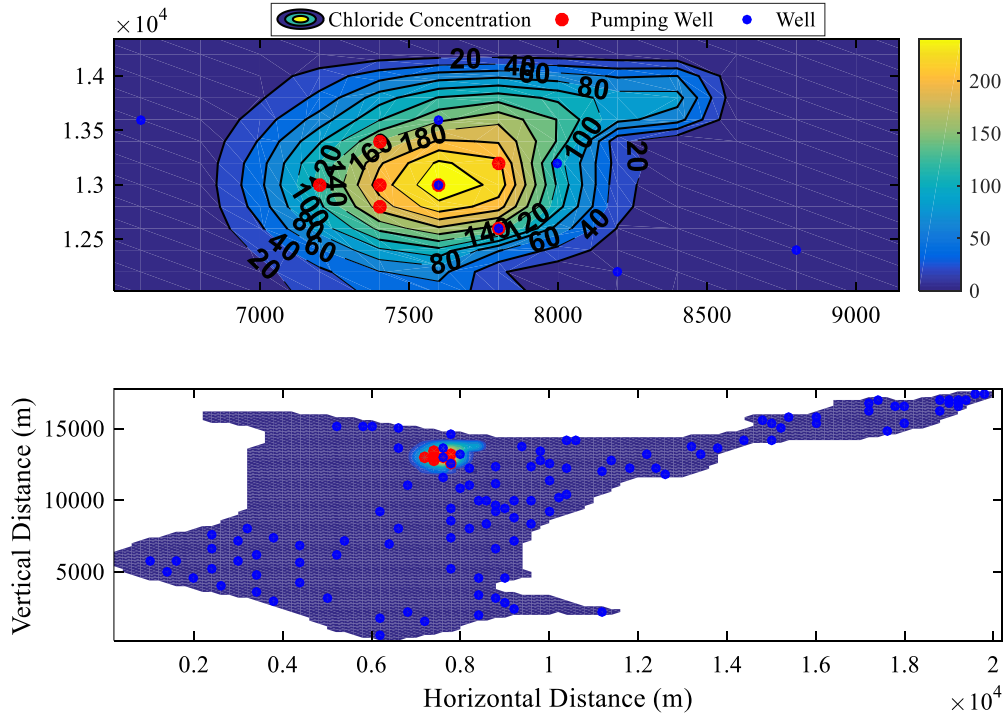

Fig. 10. The convergance trend of GA algorithm

Fig. 11. Chloride concentration distribution in Aquifer (*μg/Lit*) and pumping well locations
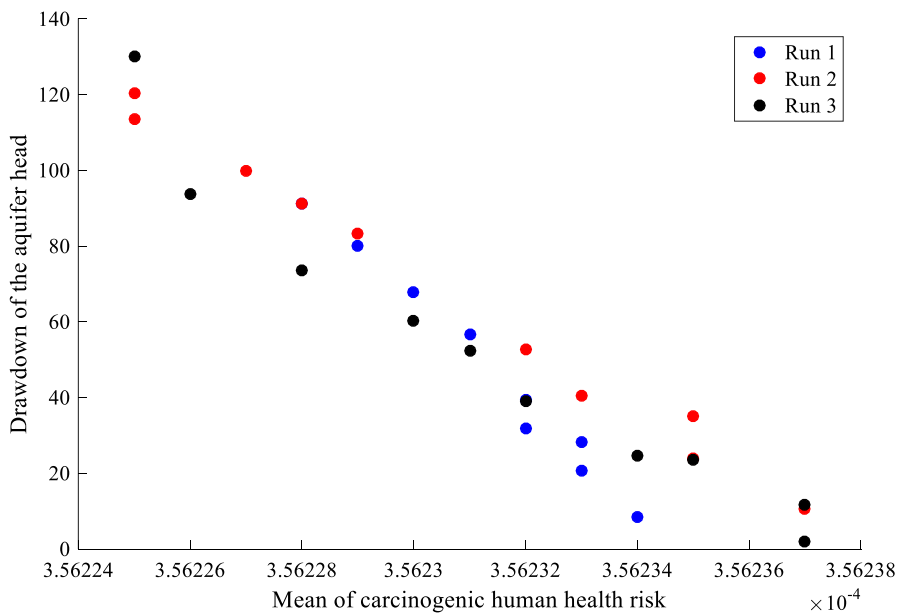

Fig. 12. Pareto fronts in NSGA-II algorithm (Seven Wells)

4. Conclusion

In this study, hybrid optimization-simulation models, GA-FEM and NSGA-II-FEM are used to solve a groundwater remediation problem by PAT method. The optimization problem with these models was solved in single-objective and two-objective cases in three scenarios. In solving the single-objective optimization problems, the objective was to determine the optimal location of three, five and seven pumping wells with a rate of 600 m³/day to minimize the mean of carcinogenic human health risk. The results indicated that the GA-FEM model has a good efficient with 356.2302×10⁻⁶, 356.2253×10⁻⁶ and 356.2226×10⁻⁶ for three scenarios, respectively. The results indicated with increases number of pumping wells amount contaminant concentration is significantly reduced. But, increasing the number of pumping wells can reduce the groundwater head and increase the risk of subsidence. So, we consider drawdown of the aquifer head as second objective function. In the two-objective

problems, the drawdown of groundwater head was also considered. The optimization problem was investigated with tree, five and seven pumping wells at a constant pumping rate of 600 m^3/day. The results indicated that among the solutions provided by each model, the most efficient solution was able to reduce the contaminant concentration in the aquifer to the standard pollutant concentrations and, conversely, to minimize drawdown of groundwater head. In general, among the Pareto-optimal solutions, the solution selected should establish a balance between the two objective functions.

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6. Disclosure Statement

No potential conflict of interest was reported by the authors

7. References

Akbarpour, A., Zeynali, M. J., & Nazeri Tahroudi, M. (2020). Locating optimal position of pumping Wells in aquifer using meta-heuristic algorithms and finite element method. *Water Resources Management*, *34*(1), 21-34.

Alexander, A. C., Ndambuki, J. M., Salim, R. W., & Manda, A. K. (2018). Groundwater remediation optimization using solving constraint integer program (scip). *Groundwater for Sustainable Development*, *7*, 176-184.

Bear, J. (1988). *Dynamics of fluids in porous media*. Courier Corporation.

Boddula, S., & Eldho, T. I. (2017). A moving least squares based meshless local petrov-galerkin method for the simulation of contaminant transport in porous media. *Engineering Analysis with Boundary Elements*, *78*, 8-19.

Darabi, B., & Ghafouri, H. (2007). Optimal identification of ground-water pollution sources.

Eldho, T. I., & Swathi, B. (2018). Groundwater Contamination Problems and Numerical Simulation. In *Environmental Contaminants* (pp. 167-194). Springer, Singapore.

Erickson, M., Mayer, A., & Horn, J. (2002). Multi-objective optimal design of groundwater remediation systems: application of the niched Pareto genetic algorithm (NPGA). *Advances in Water Resources*, *25*(1), 51-65.

Esfahani, H. K., & Datta, B. (2018). Fractal singularity–based multiobjective monitoring networks for reactive species contaminant source characterization. *Journal of Water Resources Planning and Management*, *144*(6), 04018021.

Felfli, Z., Deb, N. C., Crothers, D. S. F., & Msezane, A. Z. (2002). Angular distributions of electrons in photoionization of 3s subshell of atomic chlorine. *Journal of Physics B: Atomic, Molecular and Optical Physics*, *35*(19), L419.

Freeze, R. A., & Cherry, J. A. (1979). *Groundwater*. Prentice-hall.

Gorelick, S. M., Voss, C. I., Gill, P. E., Murray, W., Saunders, M. A., & Wright, M. H. (1984). Aquifer reclamation design: the use of contaminant transport simulation combined with nonlinear programing. *Water Resources Research*, *20*(4), 415-427.

Guneshwor, L., Eldho, T. I., & Vinod Kumar, A. (2018). Identification of groundwater contamination sources using meshfree RPCM simulation and particle swarm optimization. *Water Resources Management*, *32*(4), 1517-1538.

He, L., Xu, Z., Fan, X., Li, J., & Lu, H. (2017). Meta-Modeling-Based Groundwater Remediation Optimization under Flexibility in Environmental Standard. *Water Environment Research*, *89*(5), 456-465.

Joswig, P., Vernocchi, S., Pilone, A., Violetti, A., Brunetti, E., Pellegrini, M., ... & Grava, A. (2017). Continuously optimizing a groundwater remediation system in complex fractured media. *Università degli Studi di Cagliari*.

Kulkarni, N. H. (2015). Numerical simulation of groundwater recharge from an injection well. *International Journal of Water Resources and Environmental Engineering*, *7*(5), 75-83.

Kumar, D., Ch, S., Mathur, S., & Adamowski, J. (2015). Multi-objective optimization of in-situ bioremediation of groundwater using a hybrid metaheuristic technique based on differential evolution, genetic algorithms and simulated annealing. *Journal of Water and Land Development*, *27*, 29-40.

Mategaonkar, M., Eldho, T. I., & Kamat, S. (2018). In-situ bioremediation of groundwater using a meshfree model and particle swarm optimization. *Journal of Hydroinformatics*, *20*(4), 886-897.

Ouyang, Q., Lu, W., Hou, Z., Zhang, Y., Li, S., & Luo, J. (2017). Chance-constrained multi-objective optimization of groundwater remediation design at DNAPLs-contaminated sites using a multi-algorithm genetically adaptive method. *Journal of contaminant hydrology*, *200*, 15-23.

Sbai, M. A. (2019). Well rate and placement for optimal groundwater remediation design with a surrogate model. *Water*, *11*(11), 2233.

Seyedpour, S. M., Kirmizakis, P., Brennan, P., Doherty, R., & Ricken, T. (2019). Optimal

remediation design and simulation of groundwater flow coupled to contaminant transport using genetic algorithm and radial point collocation method (RPCM). *Science of The Total Environment*, *669*, 389-399.

Singh, A., & Minsker, B. S. (2008). Uncertainty-based multiobjective optimization of groundwater remediation design. *Water resources research*, *44*(2).

Singh, T. S., & Chakrabarty, D. (2011). Multiobjective optimization of pump-and-treat-based optimal multilayer aquifer remediation design with flexible remediation time. *Journal of Hydrologic Engineering*, *16*(5), 413-420.

Wang, H. F., & Anderson, M. P. (1995). *Introduction to groundwater modeling: finite difference and finite element methods*. Academic Press.

Wang, Y., Xiao, W. H., Wang, Y. C., Wei, W. X., Liu, X. M., Yang, H., & Chen, Y. (2018, October). Simulating-optimizing coupled method for pumping well layout at a nitrate-polluted groundwater site. In *IOP Conference Series: Earth and Environmental Science, 191*, p. 012071. IOP Publishing.

Yang, A. L., Dai, Z. N., Yang, Q., Mcbean, E. A., & Lin, X. J. (2018, May). A Multi-objective Optimal Model for Groundwater Remediation under Health Risk Assessment in a Petroleum contaminated site. In *IOP Conference Series: Earth and Environmental Science*, *146*, p. 012014. IOP Publishing.

Yang, A., Yang, Q., Fan, Y., Suo, M., Fu, H., Liu, J., & Lin, X. (2018). An Integrated Simulation, Inference and Optimization Approach for Groundwater Remediation with Two-Stage Health-Risk Assessment. *Water*, *10*(6), 694.

Younes, A., Hoteit, H., Helmig, R., & Fahs, M. (2022). A robust Upwind Mixed Hybrid Finite Element method for transport in variably saturated porous media. *Hydrology and Earth System Sciences Discussions*, 1-29.

Zeynali, M. J., Pourreza-Bilondi, M., Akbarpour, A., Yazdi, J., & Zekri, S. (2022). Optimizing pump-and-treat method by considering important remediation objectives. *Applied Water Science*, *12*(12), 268.

Zeynali, M. J., Pourreza-Bilondi, M., Akbarpour, A., Yazdi, J., & Zekri, S. (2022). Development of a contaminant concentration transport model for sulfate-contaminated areas. *Applied Water Science*, *12*(7), 169.