Optimizing pump-and-treat method by considering important remediation objectives

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Abstract
The efficiency of groundwater remediation by pump-and-treat (PAT) method is affected by several components. The most important of these components include the pumping wells location, pumping rate, and remediation period. In this research, hybrid optimization-simulation models were developed to find the appropriate groundwater remediation strategy by PAT method. The GA-FEM and NSGA-II-FEM models were used to solve four optimization problems for a hypothetical and real aquifer. These optimization problems were investigated from one objective problem to a four-objectives problem. In the multi-objective problems, in each step, one objective function is added to the previous set of objective functions. In the one-objective case, the objective function was defined as minimizing the contaminant concentration by pumping at a constant rate, while in the two-objectives problem, minimizing the drawdown of groundwater head by pumping at a constant rate was added. In the three-objectives problem, the pumping rate was variable and the mean pumping rate from all the wells is minimized. Finally, minimizing the remediation period is added in the four-objective case. The results indicated that locating the pumping wells in the path of the contaminant flow and close to the source improves the efficiency of the PAT system. The wells with higher pumping rates would be in the path of contamination flow and close to the source improves the efficiency of the PAT system. The wells with lower pumping rates should be located in nodes near the Dirichlet boundary. It is concluded that the remediation period in the hypothetical and real aquifer cannot be less than almost 3000 and 760 days, respectively. Finally, it can be said, the most important component in choosing the proper PAT strategy is the proper location of pumping wells.

Keywords Contaminant concentration · Drawdown of groundwater head · Finite element method · Genetic algorithms · Pumping rate · Remediation period

Introduction
The main groundwater contamination with anthropogenic sources consists of seepage from septic tanks, absorptive wells, and sewers, and uncontrolled hazardous waste. Declining groundwater quality and its pollution have made groundwater remediation and management an essential need. In the last few decades, groundwater contamination has become a major problem in many parts of the world reducing its availability for drinking and even agriculture. Groundwater remediation methods are very costly and time-consuming. Therefore, an efficient approach should be adopted for selecting the remediation method to eliminate the contamination efficiently. In this direction, numerical
methods and optimization tools can be very beneficial for finding the best strategy for groundwater remediation (Eldho and Swathi, 2018). In the groundwater contamination literature, some researchers have studied the pollutant sources (Ghafouri and Darabi, 2007; GuNeshwor et al., 2018) and some other researchers investigated the types of groundwater remediation methods such as groundwater phytoremediation (Kumar et al., 2015; Mategaonkar et al., 2018) or PAT method (Wang et al., 2018). Often, designing an efficient remediation system is a multi-objective task. For example, the PAT method components are concerned by the location of the pumping well, pumping rates of contaminated water, remediation period, and the drawdown of groundwater head during the remediation period.

To understand the response of the groundwater system to different remediation strategies, various numerical methods such as finite difference method (FDM) (He et al., 2017; Yang et al., 2018a), finite element method (FEM) (Ghafouri and Darabi, 2007; Esfahani and Datta, 2018), meshless method (Boddula and Eldho, 2017; Mategaonkar et al., 2018; Seyedpour et al., 2019) and software packages like MODFLOW (Singh and Chakrabarty, 2011; Joswig et al., 2017) have been used. Different methods are used to solve the groundwater remediation optimization problem. In the last decades, nonlinear programming methods (Gorelick et al., 1984) and Meta-Heuristic algorithms such as AMALGAM (Ouyang et al., 2017), probabilistic multi-objective genetic algorithm (PMOGA) (Singh and Minsker, 2008), niched Pareto genetic algorithm (NPGA) (Erickson et al., 2002) have been widely used. One of the goals of groundwater remediation is to reduce contaminant concentrations to the permissible level. The level of contaminant concentration can be directly or indirectly related to the carcinogenic human health risk (Yang et al., 2018b). Many researchers used Simulation–optimization (S–O) models for designing the process of an effective PAT system (Luo et al. 2014), (Sreekanth et al., 2016). Others minimized contaminant concentration and pumping costs, by optimizing the number of pumping wells and pumping rates (Alexander et al. 2018) and some others focused on finding the best location for pumping wells (Wang et al., 2018; Sbai, 2019) and to minimizing groundwater remediation period (Mategaonkar et al., 2018).

The purpose of this study is to find the best location for pumping wells considering the important objective functions such as minimizing contaminant concentration, minimizing the drawdown of the groundwater head, minimizing the pumping rate, and remediation period. These objectives are used in one to four objective optimization problems. The GA-FEM and NSGA-II-FEM hybrid models are used to investigate optimization problems. We combined and used FEM method with genetic algorithm for this purpose.

**Materials and methods**

**Case study**

**Hypothetical aquifer**

In this study, we consider a hypothetical aquifer. This hypothetical aquifer is almost similar to that considered by Sharif et al. (2008). The domain of this aquifer is 1800 m × 1000 m in the area as shown in Fig. 1. The hydrogeological parameters for the aquifer are presented in Table 1. The entire aquifer has a storage coefficient of 0.0004, and a landfill is considered being in Zone A with a

| Table 1 Hydrogeological aquifer data (Sharif et al. 2008) |
|----------------------------------------------------------------------------|
| Properties                | Zone A | Zone B | Zone C |
|----------------------------|--------|--------|--------|
| Porosity                   | 0.20   | 0.25   | 0.15   |
| Transmissivity $T_x$ (m$^2$/day) | 500    | 400    | 250    |
| Transmissivity $T_y$ (m$^2$/day) | 300    | 250    | 200    |
| Longitudinal Dispersivity (m) | 150    | 75     | 50     |
| Transverse Dispersivity (m) | 12.5   | 7.5    | 5.0    |
seepage rate of 0.009 m/day. It is assumed that zone A and zone C are recharged in between nodes 12–24 and 42–54 at a rate of 0.00024 and 0.00012 m/day, respectively (Fig. 1). The flow model has constant head conditions at the western and eastern boundaries with 100 and 95 m, respectively. The southern boundary is the no-flow boundary, and the aquifer is recharged only by the northern boundary at zones A and C. For the transport contaminant model, all boundaries are assumed to be impervious except the eastern boundary.

The source of contamination is a landfill. Heavy metals have leaked from this landfill for 30 years and have polluted the groundwater. One of the Important Heavy metals is chromium. The value of chromium concentration is 56 µg/Lit and based on Food and Agriculture Organization (FAO) permissible limit for chromium concentration in drinking water is 50 µg/Lit. Landfill is located on 9, 10, 15, and 16 nodes. This problem is solved using Galerkin’s finite element method and the Crank-Nicolson time scheme with a structural grid in 6 × 10 and 45 squared elements shown in Fig. 2. Distance between nodes is 200 m. Five days time step is chosen for both the groundwater flow and the contaminant transport model.

The numerical model is initialized based on the transient flow of the aquifer wherein no pumping is assumed. The entire simulation period is 30 years, with continuous contamination. The groundwater flow and the distribution of the contaminant concentrations are simulated using the finite element method. In the present case, four pumping wells are used. In the first step, the remediation period is considered 10 years. To compare the objective function value for each member of the population, we consider contaminant concentrations in eight nodes of 15, 16, 21, 22, 27, 28, 33, and 34, shown in (Fig. 2) with the square mark.

**Real aquifer**

In this study, the aquifer located in Ghaen basin is also investigated. Ghaen study area with an area of 929.1 km² 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 Mm³/ year, respectively. 0.5 Mm³ of groundwater is discharged annually from the east side of the aquifer. There is a contaminant resource with an 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 3 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 pumping wells were placed in the nearest nodes and their pumping rate was added together. Also in Table 2 the values of contaminants and their permissible limits are given. In order to use hydraulic information for aquifer modeling, 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.

**Objective functions**

PAT system costs depend on the residual contaminant concentration at the end of the remediation period. Four objective functions are considered in the hypothetical and real aquifers. These objective functions are (1) Minimizing the contaminant concentration, (2) Minimizing the drawdown of the aquifer head, (3) Minimizing the mean pumping rate, (4) Minimizing the remediation period. Therefore, the purpose
of this study is to determine the optimal location of pumping wells so that objective functions are minimized. Objective functions for four optimization problems are given in Table 3:

In the single-objective problem, we use four pumping wells at a rate of 600 m$^3$/day (pumping at a constant rate). For the two objectives problem, in addition to the first objective function, the minimization of drawdown of aquifer head with the same pumping wells at a rate of 600 m$^3$/day is considered. In the three objectives problem, the pumping rate is variable, and minimizing the mean of the pumping rate

| Contaminant        | Symbol | Unit    | Value | permissible limit |
|--------------------|--------|---------|-------|-------------------|
| Chloride           | Cl$^-$ | mg/lit  | 643.2 | 600               |
| Nitrate-Nitrogen   | NO$_3$-N | mg/lit | 19.6  | 10                |

### Table 3 Optimization problems and their Functions

| Single/multi-objective | Objective functions                                                                 |
|------------------------|--------------------------------------------------------------------------------------|
| One-objective problem  | (1) Minimizing the contaminant concentration (CC)                                     |
| Two-objectives problem | (1) Minimizing the contaminant concentration (CC) (2) Minimizing the drawdown of the aquifer head (DAH) |
| Three-objectives problem | (1) Minimizing the contaminant concentration (CC) (2) Minimizing the drawdown of the aquifer head (DAH) (3) Minimizing the mean pumping rate (MPR) |
| Four-objective problem | (1) Minimizing the contaminant concentration (CC) (2) Minimizing the drawdown of the aquifer head (DAH) (3) Minimizing the mean pumping rate (MPR) (4) Remediation period (RP) |
is also added to the set of objective functions. In the final step, considering the three previous objective functions, the remediation period is minimized. Therefore, the objective functions are defined mathematically as follows:

\[
\text{Min } F_1 = \left( \sum_{k=1}^{K} C_k \right) / K
\]  

(1)

\[
\text{Min } F_2 = \sum_{i=1}^{\text{NNODE}} (H_i^{\text{old}} - H_i^{\text{new}})
\]  

(2)

\[
\text{Min } F_3 = \sum_{j=1}^{J} q_{j}^{\text{Ex}} / J
\]  

(3)

\[
\text{Min } F_4 = \text{remediation period}
\]  

(4)

where F1 to F4 are the objective functions 1 to 4, respectively.

The first objective function minimizes the mean of contaminant concentration where K is a number of nodes and Ck is the contaminant concentration in kth nodes.

In the second objective function, the drawdown of the aquifer where, \(H_{i}^{\text{old}}\) and \(H_{i}^{\text{new}}\) are aquifer head before and after installing pumping wells at ith node, \(i\), respectively. NNODE is the total number of nodes in the aquifer domain.

The third objective function is minimizing the mean pumping rate of all wells (m³/day). J is the number of pumping wells and \(q_{j}^{\text{Ex}}\) is the pumping rate at jth pumping well (m³/day).

The fourth objective function \(F_4\) consists in minimizing the remediation period.

**Governing equations**

**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, 1982):

\[
\frac{\partial}{\partial x} \left( T_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( T_y \frac{\partial h}{\partial y} \right) = R
\]  

(5)

\[
\frac{\partial}{\partial x} \left( k_x \frac{\partial H}{\partial x} \right) + \frac{\partial}{\partial y} \left( k_y \frac{\partial H}{\partial y} \right) = R
\]  

(6)

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, 1982):

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

(7)

\[
\frac{\partial}{\partial x} \left( K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial h}{\partial y} \right) = S \frac{\partial h}{\partial t} + Q_w \delta(x - x_i)(y - y_i) - q
\]  

(8)

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]; \(S_{i}(x,y)\) is specific yield; \(Q_{w}\) is source or sink function; \((-Q_{w}=\text{source and } Q_{w}=\text{sink})\) [LT⁻¹]; \(\delta\) 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].

**FEM to solve governing equations for groundwater flow**

Using Galerkin’s finite element method and two-dimensional element for approximation Eq. 9, the first step is to define a trial solution.

\[
\hat{h}(x, y, t) = \sum_{L=1}^{\text{NP}} h_L(t) N_L(x, y)
\]  

(9)

where \(h_L\) is the unknown head, \(N_L\) is the known basis function at node \(L\), and \(\text{NP}\) 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 functions are forced to be zero and integrated over the entire domain \(\Omega\) (Desai et al, 2011). Thus, Eq. 9 can be written as:

\[
\begin{align*}
\int_{\Omega} \left[ \frac{\partial}{\partial x} \left( T_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( T_y \frac{\partial h}{\partial y} \right) - Q_w + q - S \frac{\partial h}{\partial t} \right] N_L(x, y) dx dy &= 0 \\
\sum_{e} \int_{\Omega} \left( T_x \frac{\partial \epsilon}{\partial x} \left( \frac{\partial N_L}{\partial x} \right) + T_y \frac{\partial \epsilon}{\partial y} \left( \frac{\partial N_L}{\partial y} \right) \right) dx dy &= \sum_{e} \int_{\Omega} (Q_e) N_L^e dx dy
\end{align*}
\]  

(10)

(11)

where \(\{N_L^e\} = \begin{cases} N_j & \text{for } j \leq N \cr N_j & \text{for } j > N \end{cases} \). For an element, Eq. 11 can be written in matrix form as:
\[ G^r \{ h^r_t \} + [P] \left\{ \frac{\partial h^r}{\partial t} \right\} = \{ f^r \} \]  

(12)

where I = i, j, m, n are four nodes of rectangular elements and G, P and f are the element matrices known as conductance, storage matrices, and recharge vectors, respectively. Summation of elemental matrix Eq. 12 for all the elements gives the global matrix as:

\[ [G]\{ h_I \} + [P] \left\{ \frac{h_I}{\Delta t} \right\} = \{ f \} \]  

(13)

Applying the implicit finite difference scheme for \( \frac{\partial h}{\partial t} \), term in time domain for Eq. 13 gives.

\[ [G]\{ h_I \}_{t+\Delta t} + [P] \left\{ \frac{h_{I+\Delta t} - h_I}{\Delta t} \right\} = \{ f \} \]  

(14)

The subscripts t and t + Δt represent the groundwater head values at earlier and present time steps. By rearranging the terms of Eq. 14, the general form of the equation can be given as (Desai et al. 2011):

\[ \{P\} + \omega \Delta t [G] \{h\}_{t+\Delta t} = \{P\} - (1 - \omega) \Delta t [G] \{h\}_t + \Delta t (1 - \omega) \{f\}_t + \omega \{f\}_{t+\Delta t} \]  

(15)

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 \( \omega = 1 \).

### 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 (Ghafouri and Darabi, 2007):

\[
\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(D_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y} \left(D_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z} \left(D_z \frac{\partial C}{\partial z}\right) - \nu_x \frac{\partial C}{\partial x} - \nu_y \frac{\partial C}{\partial y} - \nu_z \frac{\partial C}{\partial z} + \text{CHEM}
\]  

(16)

Equation 16 is three-dimensional governing equation of advection–dispersion of contaminants in groundwater resources where \( R = 1 + \frac{\nu^2}{\theta} \) is the retardation factor with \( \rho_b \) = media bulk density \([\text{ML}^{-3}]\), and \( K_a \) = sorption coefficient \([\text{L}^3\text{M}^{-1}]\); C(x,y,t) is solute concentration \([\text{ML}^{-3}]\); \( D_x \) and \( D_y \) are components of dispersion coefficient tensor \([\text{L}^2\text{T}^{-1}]\); \( \lambda \) is the reaction rate constant \([\text{T}^{-1}]\).

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

\[ h(x, y, 0) = h_0(x, y); C(x, y, 0) = f \quad x, y \in \Omega \]  

(21)

The flow and transport equations should be solved with appropriate boundary conditions. The boundary conditions can be written as follows (Eldho and Swathi 2018):

\[ h(x, y, t) = h_1(x, y, t); C(x, y, t) = g_1 \quad x, y \in \Gamma_1 \]  

(22)

\[ \frac{q}{q_{\text{in}}} = q_1(x, y, t) \]  

for the confined aquifer, \( K \frac{\partial h}{\partial x} = q_2(x, y, t) \) is for unconfined aquifer.
where \( \Omega \) is flow region; \( I = I_1 \cup I_2 \) is region boundary; \( \frac{\partial}{\partial n} \) is normal derivative; \( h_0(x,y) \) is the initial head in the flow domain \([L]\); \( h_1(x,y,t) \) is the known head value at the boundary section \( \Gamma_1[L] \); \( f \) is a given function in \( \Omega \), \( g_1 \) and \( g_2 \) are given functions along boundary sections \( \Gamma_1 \) and \( \Gamma_2 \); and \( n_x, n_y \) are the components of the unit outward normal vector to the boundary section \( \Gamma_2 \).

\[
(D_x \frac{\partial C}{\partial x}) n_x + (D_y \frac{\partial C}{\partial y}) n_y = g_2 \quad x, y \in \Gamma_2
\]  

(23)

where \( \Omega \) is flow region; \( I = I_1 \cup I_2 \) is region boundary; 
\( \frac{\partial}{\partial n} \) is normal derivative; \( h_0(x,y) \) is the initial head in the flow domain \([L]\); \( h_1(x,y,t) \) is the known head value at the boundary section \( \Gamma_1[L] \); \( f \) is a given function in \( \Omega \), \( g_1 \) and \( g_2 \) are given functions along boundary sections \( \Gamma_1 \) and \( \Gamma_2 \); and \( n_x, n_y \) are the components of the unit outward normal vector to the boundary section \( \Gamma_2 \).

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 with a variety of element types and number of nodes. The elements join together and then, the 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 (Ghafouri and Darabi 2007):

\[
[C]_{t}^{i+\Delta t} = [B][C]_{t} + [f]
\]  

(25)

where:

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

(26)

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

(27)

\( \Delta t \) is the length of time interval, the so-called time-step. \([C]_{t}^{i} \) is the vector of known concentrations at the beginning of any the time step and \([C]_{t}^{i+\Delta t} \) is the vector of sought unknown concentrations at the end of time step. \([G]\), \([U]\), \([F]\) and \([P]\) are square matrices in which the number of rows and columns are equal to the number of nodal points in the computational grid. The elements of these matrices are computed as follows (Ghafouri and Darabi 2007):

\[
G_{e}(L,i) = -\int_{e} \left(D_x \frac{\partial N^e_i}{\partial x} \frac{\partial N^e_L}{\partial x} + D_y \frac{\partial N^e_i}{\partial y} \frac{\partial N^e_L}{\partial y} + D_z \frac{\partial N^e_i}{\partial z} \frac{\partial N^e_L}{\partial z} \right) dxdydz
\]  

(28)

\[
P_{e}(L,i) = \int_{e} R N^e_i N^e_L dxdydz
\]  

(29)

\[
U_{e}(L,i) = -\int_{e} \left(V_{x} \frac{\partial N^e_i}{\partial x} N^e_L + V_{y} \frac{\partial N^e_i}{\partial y} N^e_L + V_{z} \frac{\partial N^e_i}{\partial z} N^e_L \right) dxdydz
\]  

(30)

\[
F_{e}(L,i) = -\int_{e} R \lambda N^e_i N^e_L dxdydz
\]  

(31)
$\{f\}$ is the load vector calculated using the following boundary integral:

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

(32)

where $\hat{c}$ denotes the given concentration values at boundary nodes, $n_i$ is directional cosines and $\Gamma$ is the domain boundary.

---

Fig. 5 Groundwater head and Chromium concentration distribution

(a) Groundwater Head after 30 Years

(b) Chromium Concentration Distribution after 30 Years (mg/lit)

Table 4 Statistical characteristics of the GA performance

| Algorithm | The best value | The worst value | Average values |
|-----------|----------------|----------------|---------------|
| GA        | 41.79331       | 41.79361       | 41.79355      |

GA and NSGA-II algorithms

In the genetic algorithm (GA) and its multi-objective version (Non-Dominated Sorting Genetic Algorithm, NSGA-II), there are crossover and mutation phases. In the single-objective version, the 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). So, in the NSGA-II algorithm, the members of the population who are in the first front are certainly better than the members of the second front and
1. Chain constraints (sequential selection)

In the hypothetical aquifer, we consider four pumping wells with the pumping rate of 600 m$^3$/day. The aquifer was gridded with 60 nodes as shown in Fig. 2. In this case, it is not possible to select the boundary nodes as a pumping well location. Therefore, in the first step, these nodes are removed from the set of 60 nodes. Now, given the assumed aquifer geometry and the number of boundary nodes, the number of nodes able to select as pumping wells will be 32 nodes.
After that, each time a pumping well is added to the aquifer, the node in which the pumping well is located and the nodes in the capture zone are removed from the set of selectable nodes.

Results and discussion

The results of hypothetical aquifer modeling

The hypothetical aquifer has been investigated using FEM and rectangular element. The results of groundwater flow and contaminant transport modeling for 30 years are presented in Fig. 5a and 5. As discussed in the preceding section, the hypothetical aquifer is considered with no pumping wells. The landfill is the source of contaminants.

The results of one-objective optimization problem (hypothetical aquifer)

The one-objective optimization problem is solved to find the pumping wells’ location in order to obtain optimum (near-optimum) values for the first objective function. It should be noted that the first step in all remediation systems is removing pollutant sources or avoiding their dissemination and then pumping wells are installed. In this study after preventing seepage from the landfill, the contaminated groundwater is pumped by the wells, for 10 years.

Population size and maximum iteration for genetic algorithms were 10 and 20, respectively, the genetic algorithm was run five times. The results of the five runs of GA, including the best, the worst and mean values of the objective function in the five runs are presented in Table 4. As can be seen in this table, the genetic algorithm has a good performance with an average amount of first objective function equal to 41.7935 (µg/Lit). The best performance of GA is also shown in Fig. 6.
Fig. 10  a Groundwater head, b contaminant concentration

Fig. 11  Pareto front of NSGA-II algorithm in four objective functions
Table 5  Comparison of solutions with the minimum of each objective function

| Objective function | 1st O.F. (CC) | 2nd O.F. (DAH) | 3rd O.F. (MPR) | 4th O.F. (RP) |
|--------------------|---------------|----------------|----------------|---------------|
| Min O.F. one       | 41.493        | 65.971         | 561.956        | 597           |
| Min O.F. two       | 41.590        | 58.041         | 549.114        | 638           |
| Min O.F. three     | 41.588        | 61.658         | 527.765        | 638           |
| Min O.F. four      | 41.493        | 65.971         | 561.956        | 597           |

Fig. 12  Groundwater head and contaminant distribution after 5 years
The pumping well location, with 600 m$^3$/day, (solid circle marker) and the concentration of Chromium in the aquifer domain after optimization during ten years of remediation are shown in Fig. 7. As can be seen in this figure, the best location of pumping wells is contaminant movement path. When the contamination mass is moving to the right of the aquifer, the algorithm located two more wells in front of that to remove most of the contaminants. With a constant rate of pumping (600 m$^3$/day) and the shown location of pumping wells, the concentration of contamination throughout the aquifer is reduced to the permissible level.

The results of two-objective optimization problem (hypothetical aquifer)

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 five times. The number of solutions in the Pareto-optimal front for run 1 to run 5 are 6, 10, 5, 8 and 10, respectively. The results of all runs are shown in Fig. 8.

As it can be seen in this figure, NSGA-II algorithm finds the solution with a minimum of the first objective function in run 3 and 5. Also, NSGA-II algorithm finds the solution with a minimum of the second objective function in run 4. But, we can consider run 2 as the best performance of NSGA-II algorithm. Because this run of NSGA-II algorithm has good coverage on solution space. Also, run 2 could find the minimum for two objective functions.

The results of three-objective optimization problem (hypothetical aquifer)

In Three-Objective optimization problem, we find the best location of wells to find the minimum of contaminant concentrations, the drawdown of the aquifer head and mean pumping rate. In this problem, NSGA-II algorithm is run five times and the solutions in the Pareto front for run 1 to run 5 are 10, 9, 10, 10 and 10, respectively. The results of NSGA-II algorithm indicate that the number of solutions in the Pareto-fronts for NSGA-II algorithm is higher than in the case of the two-objective optimization problem. In this case, the algorithm is able to get any value as a pumping rate in a range of [500,600]. In Fig. 9, the Pareto front of NSGA-II algorithm in the last run is shown.

For the chosen solution that is shown in red color in Fig. 9, the pumping rates of four pumping wells are 553.4, 579.4, 558.6 and 558.2 m$^3$/day, respectively. The location of pumping wells in the groundwater head and contaminant concentration is shown in Fig. 10. As shown in this figure, two wells with higher pumping rates are located close to in the contaminant source, but one of them is located close to the left boundary (constant head boundary), thus, in addition to minimizing contaminant concentration, the drawdown of groundwater head will also be minimized.

The results of four-objective optimization problem (hypothetical aquifer)

In four-objective optimization problem, we find the best location of wells to find the minimum of contaminant concentrations, the drawdown of the aquifer head, mean pumping rate and the maximum concentration of Chromium. In this problem, NSGA-II algorithm is run five times and the solutions in the Pareto front for run 1 to run 5 are 10, 10, 10, 10 and 10, respectively. The results of NSGA-II algorithm indicate that the number of solutions in the Pareto-fronts for NSGA-II algorithm is higher than in the case of the three-objective optimization problem. In this case, the algorithm is able to get any value as a pumping rate in a range of [500,600]. In Fig. 11, the Pareto front of NSGA-II algorithm in the last run is shown.

For the chosen solution that is shown in red color in Fig. 11, the pumping rates of four pumping wells are 553.4, 579.4, 558.6 and 558.2 m$^3$/day, respectively. The location of pumping wells in the groundwater head and contaminant concentration is shown in Fig. 12. As shown in this figure, two wells with higher pumping rates are located close to in the contaminant source, but one of them is located close to the left boundary (constant head boundary), thus, in addition to minimizing contaminant concentration, the drawdown of groundwater head will also be minimized.
concentrations, the drawdown of the aquifer head, mean pumping rate and remediation period.

In the last step, the optimization problem with four-objective functions is also investigated. In single-objective to three-objective problems, the remediation period was equal to 10 years. The fourth objective function is the remediation period minimization.

Population size and maximum iteration for NSGA-II algorithm were 10 and 20, respectively. NSGA-II algorithm was run five times. The results of the second run of NSGA-II
The results of real aquifer modeling

The real aquifer has been investigated using FEM and rectangular element. The results of groundwater flow and Chloride transport modeling for 5 years are presented in Fig. 12a and b. The real aquifer is considered with pumping wells.

The results of one-objective optimization problem (real aquifer)

One-Objective optimization problem is solved to find the pumping wells’ location in order to obtain optimum (near-optimum) values for the first objective function. In this case, the contamination concentration affects only a small part of the aquifer. Therefore, it is not necessary to explore the entire aquifer domain. As heuristic information, we limited the search domain to determine the best location of the pumping wells. The new search domain
is around contaminant distribution. Therefore, members of the population in the genetic algorithm search only a domain 1600 × 2200 m. The new study domain is a structural grid in 12 × 9 and 88 squared elements. The distance between nodes is 200 m. Also, we amused 20 nodes around the contaminant source for calculating the first objective function. The remediation period is considered 3 years after preventing contaminant seepage. Monitoring nodes were also considered around the contaminant source. Population size and maximum iteration for genetic algorithms were 10 and 20, respectively. The results of GA are shown in Fig. 13.

The pumping wells’ location, with 800 m³/day, (red circle marker) and the concentration of Nitrate-Nitrogen in the aquifer domain after optimization during 3 years of remediation are shown in Fig. 14. As can be seen in this figure, the best location of pumping wells where the concentration of pollutant is maximum at the beginning of the remediation period and a round of that point. When the contamination mass is moving to the right of the aquifer, the algorithm located one well in front of that to remove most of the contaminants. But there is pumping well for agricultural use in this location. Therefore, in multi-objective problems, nodes in which there are wells for agricultural use, similar to nodes located at the aquifer boundary, are removed from the selectable nodes.

**The results of two-objective optimization problem (real aquifer)**

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 this case, the nodes with pumping wells for agriculture use is not in selectable nodes set. The parameter of NSGA-II in the real case studies is the same hypothetical case studies. The number of solutions in the Pareto-optimal front was 9. The results of these runs are shown in Fig. 15.

After that, we selected one of the solutions in optimal pareto-front. Groundwater flow and Nitrate-Nitrogen concentration for this solution are shown in Fig. 16a and b, respectively.

**The results of three-objective optimization problem (real aquifer)**

In Three-Objective optimization problem, we find the best location of wells to find the minimum of contaminant concentrations, the drawdown of the aquifer head and mean...
pumping rate. In this case, NSGA-II algorithm is able to get any value as a pumping rate in a range of [500,800]. In Fig. 17, the Pareto front of NSGA-II algorithm is shown.

The results of four-objective optimization problem (real aquifer)

In four-objective optimization problem, we find the best location of wells to find the minimum of contaminant concentrations, drawdown of the aquifer head, mean pumping rate and remediation period.

Population size and maximum iteration for NSGA-II algorithm was 10 and 20, respectively. The results of NSGA-II algorithm is shown in Fig. 18. Each solution is shown as a solid curve in two-dimensional space, and the 3rd dimension (drawdown of the aquifer head) is shown by the size of the curve and the 4th dimension (remediation period) is shown by the color bar graph. Each of these solutions can be a groundwater remediation alternative for the PAT system. As shown in this figure and due to $\Delta T = 5$ days, changing the remediation policy from one option to another can reduce the remediation period by almost 50 days without exceeding the permissible limit of contaminant concentrations at the end of the remediation period.

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 hypothetical aquifer was almost similar to the aquifer considered by Sharif et al. 2008. The optimization problem with these models was solved in single-objective and multi-objective cases. In solving the single-objective optimization problem, the objective was to determine the optimal location of four pumping wells with a rate of 600 m$^3$/day to minimize the mean of contaminant concentration. The results indicated that the GA-FEM model has a good efficiency with 41.79 ($\mu$g/Lit) and 126.04 (mg/lit) for a hypothetical and real case study, respectively. In the two-objectives problem, the drawdown of groundwater head was also considered. The optimization problem was investigated with four pumping wells at a constant pumping rate of 600 m$^3$/day. The results indicated that the number of solutions in the Pareto front was not high, due to the constant pumping rate and a low number of selectable nodes in aquifer the domain. However, 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, minimize the drawdown of groundwater head. In general, among the Pareto-optimal solutions, the solution selected should establish a balance between the two objective functions.

When considering the three-objectives optimization problem, and given of the possibility of selecting any value for the pumping rate of wells, solutions in the Pareto front were more than the two-objective problem. In some cases, even the entire population of the NSGA-II-FEM model appeared in the Pareto front. In the last step, four-objectives problem was also examined, in which the fourth objective function was minimizing the remediation period. The results of this section indicated that by changing the PAT policy, the remediation period can be reduced to 7 and 2 months for the hypothetical and real case study, respectively, without exceeding the permissible amount of pollutants at the end of the remediation period.

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Declarations

Conflict of interest There is no conflict of interest in this research.

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