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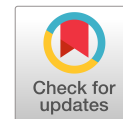
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Optimal In Situ Bioremediation Design of Groundwater Contaminated with Dissolved Petroleum Hydrocarbons

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Abstract: Aquifers are one of the main water supply resources for drinking, agricultural, and industrial purposes. Therefore, it is crucial to study and evaluate different remediation methodologies that can be used to enhance the quality of groundwater. In situ bioremediation is one of the most efficient and cost-effective cleanup methodologies to treat groundwater pollution. This methodology relies on the microorganisms of a contaminated aquifer to treat polluted groundwater. This paper presents a multiobjective simulation-optimization (S-O) model to achieve the best in situ bioremediation system design for a groundwater with contaminated dissolved hydrocarbons. Minimizing the design and operational costs along with the sum of squared cleanup standard violations (SCSV) are the two main objectives of this study. The results of optimization are presented in the form of Pareto possibility frontiers. A model from the literature and a nondominated sorting genetic algorithm are used for groundwater simulation and optimization, respectively, in this work. Single-objective and multiobjective cleanup optimized designs were obtained. The results of the single-objective design confirmed the capability and accuracy of the developed S-O model. The multiobjective optimization results yielded a Pareto frontier that can be used by regulators to select the best design tradeoff between the cleanup standard requirements and the financial resources. For example, an optimal option that reduces total cost about 51.3% increases the SCSV about 1.9%. Moreover, the option that increases the SCSV by about 12.6% decreases the total cost equal to 76.2%. A sensitivity analysis was performed for some of the bioremediation parameters such as hydraulic conductivity, initial oxygen concentration, injected oxygen concentration, remediation time, and the ratio of oxygen to hydrocarbon consumed. The results show that the hydraulic conductivity and remediation time had the most impact on the effectiveness of the bioremediation operation. DOI: 10.1061/(ASCE)HZ.2153-5515.0000304. © 2015 American Society of Civil Engineers.

Author keywords: Groundwater; In situ bioremediation; Multiobjective; Sum of squared cleanup standard violations; Sensitivity analysis.

Introduction

Recent publications dealing with newly-developed optimization models cover several domains of water resources systems, such as reservoir operation (Ashofteh et al. 2013b, 2015a, c), design and operation of pumped-storage and hydropower systems (Bozorg Haddad et al. 2014), levee layouts and design (Bozorg Haddad et al. 2015b), hydrology (Ashofteh et al. 2013a), qualitative management of water resources systems, (Bozorg Haddad et al. 2015a), and algorithmic developments (Ashofteh et al. 2015b). However, only a few of these models focus on the optimal in situ ground water remediation planning.

The high cost of designing and operating groundwater remediation systems has prompted researchers to search for and develop optimization methods for finding designs with the best performance and the lowest costs. Extraction of groundwater and its subsequent treatment in special plants (pump-and-treat) is a

common ex situ method for groundwater remediation. After treatment, the treated effluent is returned to surface water bodies, passed through conventional sewage plants, or injected into the subsurface. Pump-and-treat is a promising method for groundwater remediation when conditions allow it. Its performance has been investigated in several studies, and successful applications have been documented.

Kuo et al. (1992) used the simulated annealing algorithm for optimizing a pump-and-treat system. Guan and Aral (1999) proposed a progressive genetic algorithm (PGA), to solve nonlinear optimization problems in groundwater remediation design. Mylopoulos et al. (1999) developed a stochastic optimization method for the remediation design of a contaminated groundwater with limited hydrologic information. The performance of proposed algorithm was effectively confirmed in a case study of the Kalamaria aquifer, Chalkidiki, Greece. Aly and Peralta (1999) presented a simulation-optimization model for solving single and multiple planning-period problems in groundwater remediation. These authors also compared the performance of formal mixed-integer nonlinear programming and a genetic algorithm (GA) for several optimization scenarios. The results demonstrate an acceptable efficiency of the proposed method. Papadopolou et al. (2004) studied the effect of economic parameters on the optimal design of groundwater remediation systems. Hilton and Culver (2005) used three versions of genetic algorithms for optimal design of a groundwater remediation system with unknown parameters. Their results indicated that the robust genetic algorithm performed well for optimal design of pump-and-treat remediation systems. Sinha and Minsker (2007) proposed multiscale island injection genetic algorithms for solving optimal designs of groundwater remediation for field-scale problems of high computational complexity. This

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approach was tested using a field scale pump-and-treat design problem at the Umatilla Army Depot in Oregon. Yan and Minsker (2011) presented an approach for replacing a large number of Monte Carlo simulations with surrogate models within a noisy genetic algorithm. The surrogate models used in this study were artificial neural network (ANN). Their approach was successfully applied to a field-scale groundwater remediation case study. The results of this approach are more accurate than those of GA with lower computational requirements.

Although pump-and-treat is a relatively well-established groundwater remediation technology, it has disadvantages. Among the latter are (1) clean water is mixed with contaminated groundwater while pumping, (2) limited effectiveness in multilayered and heterogeneous aquifers, and (3) there may be high costs for groundwater extraction and construction/operation of above-ground treatment facilities. For these reasons, increased attention and research has been given to bioremediation of groundwater, especially that which has been contaminated with dissolved petroleum hydrocarbons. In a bioremediation system, the contaminants are biodegraded to harmless byproducts.

A groundwater bioremediation system is applicable either ex situ or in situ. Ex situ bioremediation systems are implemented above ground while in situ bioremediation systems are deployed in the subsurface. In situ bioremediation systems enrich water with different stimulants such as oxygen or other oxidants and inject it into the subsurface with injection wells. Soil microorganism biodegrade the groundwater contaminants into harmless products aided by the blended stimulants. Low cost and high removal efficiency are important advantages of using in situ bioremediation to clean up contaminated groundwater (Cookson 1995; Sturman et al. 1995).

Minsker and Shoemaker (1998a, b) presented a coupled optimal control and simulation model to determine the location of extraction and injection wells and the pumping rates in cost-effective in situ bioremediation. Yoon and Shoemaker (1999) used eight optimization algorithms to identify the most cost-effective in situ bioremediation design and identified an algorithm with the best combination of efficiency and accuracy. Liu and Minsker (2004) developed a full multi scale optimization approach to solve partial differential equation (PDE) constrained in situ bioremediation design. The developed approach significantly decreased the computational time in comparison with the single-grid model. Shieh and Peralta (2005) reported a simulation-optimization model that combined the genetic algorithm and simulated annealing algorithm for searching optimal solution and applied the *BIOPLUME II* model to simulate in situ bioremediation and hydraulic conditions. This approach introduced parallel recombinatory simulated annealing (PRSA) and tested its performance successfully. Prasad and Mathur (2008) applied a neural-network-embedded Monte Carlo approach to determine the potential well locations for in situ bioremediation of contaminated groundwater. Mategaonkar and Eldho (2012) developed a simulation-optimization model to determine the optimal design of an in situ bioremediation design. *BIOPLUME II* was applied to simulate the in situ bioremediation system, and the mesh-free point collocation method (PCM) was applied to solve the transport equations. The particle swarm optimization (PSO) algorithm solved for injection rates as decision variables. The results of this model were compared with those of FEM and demonstrated the efficiency of this model.

There are several studies that applied multiobjective optimization algorithms in groundwater remediation design. Erickson et al. (2002) applied the niched Pareto genetic algorithm (NPGA) to solve groundwater remediation problems with a pump-and-treat system that minimized the remedial design cost and the

contaminant mass remaining at the end of the remediation. The applied method effectively found the optimal solutions. Ren and Minsker (2005) applied the nondominated sorting genetic algorithm II (NSGA II) to optimize groundwater remediation systems. Their algorithm minimized the total cost, health risk, and the total cleanup time. Singh and Minsker (2008) proposed an approach for multiobjective optimization introduced probabilistic multiobjective genetic algorithm (PMOGA). Mondal et al. (2010) developed a simulation-optimization model incorporating the finite-element method for modeling of groundwater flow and contaminant transport with NSGA II for optimization of groundwater bioremediation in India. Singh and Chakrabarty (2011) coupled the groundwater flow model modular three dimensional finite difference groundwater flow model (MODFLOW) and the contaminant transport model modular three dimensional multi-species transport model for simulation (MT3DMS) with NSGA II. The performance of this new technique was demonstrated with three remediation design scenarios in a hypothetical multilayer confined aquifer under steady-state flow conditions.

Review of the groundwater remediation literature indicates that many studies have applied the pump-and-treat (PAT) method for remediating contaminated groundwater. Familiarity with PAT and available technologies explain much of its popularity. On the other hand, the number of field studies applying in situ bioremediation is small compared with PAT applications. This could be due to the novelty of in situ bioremediation compared to PAT. There are at present many laboratory studies being pursued to evaluate the performance and efficiency of different approaches for in situ bioremediation. Also, a few studies have combined PAT and in situ bioremediation. The first such study was that by Shieh and Peralta (2005), whose results indicate that combining these two technologies performs better than implementing them individually.

In this study, a multiobjective simulation-optimization (S-O) model is applied to find optimum in situ bioremediation designs for groundwater contaminated with dissolved petroleum hydrocarbons. Specifically, a novel two-objective optimization problem is solved that minimizes the total cost of the bioremediation project and minimizes the SCSV. The results of this optimization problem are presented as an optimum Pareto boundary. *BIOPLUME II* is applied for simulation of the in situ bioremediation system and NSGA II is used for its optimization. Another innovation of this work is linking the simulation software and optimization algorithm in *MATLAB*. This linkage allows all optimization algorithms written in *MATLAB* to solve an in situ bioremediation problem. Fig. 1 shows the flow-process diagram of the methodology applied in this paper. According to Fig. 1, the case study is simulated by determining initial values of simulation model parameters and initial random population. After that, objective functions values are calculated based on the output of the simulation model. At this stage, the optimization process (dotted box) is started and optimal solutions are calculated with an iterative search process. The following sections describe the paper's method and its implementation

Methods

Simulation of Dissolved Petroleum Hydrocarbons with BIOPLUME II

The *BIOPLUME II* model is applied to simulate bioremediation of groundwater contaminated with dissolved hydrocarbons. The transport of dissolved hydrocarbons is simulated by a two-dimensional model (2D) governed by an oxygen-limited biodegradation process. *BIOPLUME II* computes the concentration of hydrocarbons

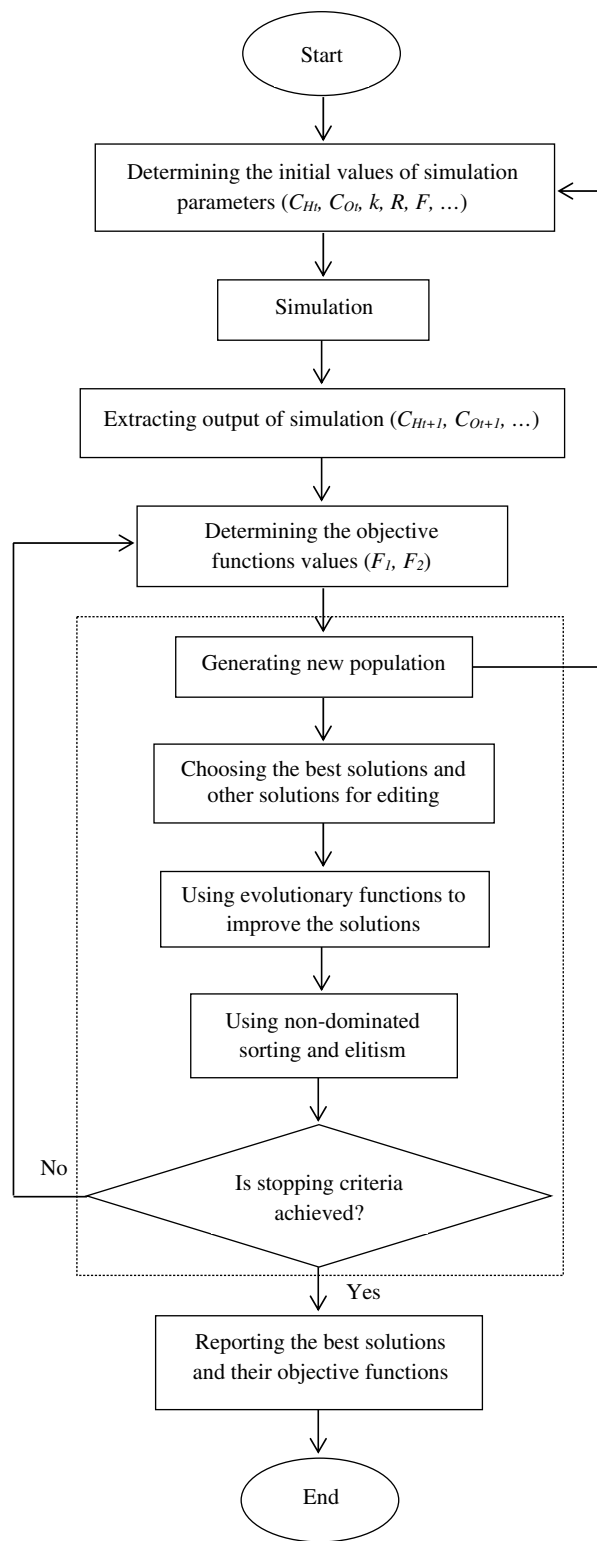


Fig. 1. Flowchart of the methodology

dissolved in groundwater during remediation. The changes in the concentration of the contaminants are affected by four distinct processes: (1) convection transport, (2) hydrodynamic dispersion, (3) fluid sources or sinks, and (4) reactions.

Borden and Bedient (1986) presented the theoretical basis of *BIOPLUME II*. The growth of microorganisms and the removal of hydrocarbon and oxygen in the aquifer are simulated using a modified Monod function

$$\frac{dC_H}{dt} = -C_{M_T} \cdot K \cdot \frac{C_H}{(K_H + C_H)} \cdot \frac{C_O}{(K_O + C_O)} \quad (1)$$

$$\frac{dC_O}{dt} = -C_{M_T} \cdot K \cdot F \cdot \frac{C_H}{(K_H + C_H)} \cdot \frac{C_O}{(K_O + C_O)} \quad (2)$$

$$\frac{dC_{M_T}}{dt} = C_{M_T} \cdot K \cdot Y \cdot \frac{C_H}{(K_H + C_H)} \cdot \frac{C_O}{(K_O + C_O)} + K_{OC} \cdot Y \cdot C_{OC} - b \cdot C_{M_T} \quad (3)$$

where C_H = hydrocarbon concentration (ML^{-3}); dC_H/dt = hydrocarbon concentration gradient at time t ; C_{M_T} = total microbial concentration (ML^{-3}); C_O = oxygen concentration (ML^{-3}); t = time (T); K = maximum rate of hydrocarbon utilization per unit mass of microorganisms; K_H = hydrocarbons half-saturation constant; K_O = oxygen half-saturation constant; dC_O/dt = oxygen concentration gradient in time t ; F = ratio of oxygen to hydrocarbon consumed (dimensionless); dC_{M_T}/dt = total microbial concentration gradient at time t ; Y = microbial yield coefficient (dimensionless); K_{OC} = first-order decay rate of natural organic carbon; C_{OC} = natural organic carbon concentration (ML^{-3}); and b = microbial decay rate.

Bear (1979) combined Eqs. (1) and (2) for removing oxygen and hydrocarbons with the advection–dispersion equations for a solute with linear instantaneous adsorption and obtained the following equations:

$$\frac{\partial C_H}{\partial t} = \frac{\nabla(D_s \cdot \nabla C_H - v_s \cdot C_H)}{R_H} - \frac{C_{M_T} \cdot K}{R_H} \cdot \frac{C_H}{(K_H + C_H)} \cdot \frac{C_O}{(K_O + C_O)} \quad (4)$$

$$\frac{\partial C_O}{\partial t} = \nabla(D_s \cdot \nabla C_O - v_s \cdot C_O) - C_{M_T} \cdot K \cdot F \cdot \frac{C_H}{(K_H + C_H)} \cdot \frac{C_O}{(K_O + C_O)} \quad (5)$$

where D_s = dispersion hydrodynamic coefficient tensor (L^2T^{-1}) in the direction s ; v_s = Darcy velocity (LT^{-1}) in the direction s ; and R_H = retardation factor defined as the ratio of the average linear velocity of groundwater to the velocity of the contaminant (Wetzelhuetter 2013) (dimensionless).

BIOPLUME II assumes that the exchange of microorganisms between the soil surface and the free solution is linearly related to the total microorganism concentration. The movement of microorganisms is simulated applying the retardation factor method (Freeze and Cherry 1979)

$$\frac{\partial C_{M_s}}{\partial t} = \frac{\nabla(D_s \cdot \nabla C_{M_s} - v_s \cdot C_{M_s})}{R_M} + C_{M_s} \cdot K \cdot Y \cdot \frac{C_H}{(K_H + C_H)} \cdot \frac{C_O}{(K_O + C_O)} + \frac{K_{OC} \cdot Y \cdot C_{OC}}{R_M} - b \cdot M_s \quad (6)$$

$$C_{M_a} = K_M \cdot C_{M_s} \quad (7)$$

$$C_{M_T} = C_{M_s} + C_{M_a} = (1 + K_M) \cdot C_{M_s} = R_M \cdot C_{M_s} \quad (8)$$

where C_{M_s} = concentration of microbes in solution (ML^{-3}), C_{M_a} = concentration of microbes attached to solids (ML^{-3}), K_M = ratio of microbes attached to microbes in solution (dimensionless), and R_M = microbial retardation factor (dimensionless).

In addition, the hydrocarbon and oxygen utilization by micro-organisms in the body of plume can be approximated as an instantaneous reaction between hydrocarbon and oxygen (Rifai and Bedient 1990). This approximation is written as an explicit finite-difference form in the following equations:

$$C_{H_{t+1}} = C_{H_t} - C_{O_t}/F \quad C_{O_{t+1}} = 0 \quad \text{If } C_{H_t} > C_{O_t}/F \quad (9)$$

$$C_{O_{t+1}} = C_{O_t} - C_{H_t} \cdot F \quad C_{H_{t+1}} = 0 \quad \text{If } C_{O_t} > C_{H_t} \cdot F \quad (10)$$

where C_{H_t} and $C_{H_{t+1}}$ = hydrocarbon concentration at times t and $t + 1$, respectively; and C_{O_t} and $C_{O_{t+1}}$ = oxygen concentrations at times t and $t + 1$, respectively.

Nondominated Sorting Genetic Algorithm (NSGA) II

The NSGA II was introduced by Deb et al. (2002), and thereafter used by researchers in various scientific disciplines. This method is based on the genetic algorithm (GA), nondominated sorting, and elitism.

GAs

Genetic algorithms were first introduced by Holland (1975). This method is based on Darwin's theory of evolution and proposed that organisms are best able to survive in a changing environment that is the most stable among all probable ones. This algorithm starts with an initial set of randomly-selected solutions and introduces an initial population. The population is made up of a number of chromosomes, where each of one is a possible answer to the optimization problem. Each chromosome is made up of a series of genes that are decision variables. The population size is the key factor in the ability of the GA to achieve an optimal solution.

Two types of operators are used in GA: (1) evolutionary operators, such as selection, and (2) genetic operators such as crossover and mutation. The selection process is based on the objective-function value corresponding to each chromosome in each generation. Policies used for the selection of the best chromosome and transport it to the next generation are (1) the roulette wheel, and (2) tournament selection (Shokri et al. 2013).

Nondominated Sorting

If a multiobjective optimization problem has an optimal solution i with respect to all objectives, then any nonoptimal solution j is dominated by the solution i . But if at least one of the objective functions has solution j better than solution i , then neither solutions i or j have an advantage over each other, and the i and j solutions are called nondominated relative to each other.

In the NSGA II, the nondominated solutions of each generation constitute a set of solutions that are best solutions in that generation. This set is called the first-rank nondominated solutions. In the next stage, the first-rank nondominated solutions are excluded and the set of nondominated solutions among remaining solutions are called second-rank nondominated solutions. By following this process, the total population of each generation is ranked and a nondominated sequence with different rankings is formed.

Elitism

The concept of elitism in the NSGA II means that the parent and child generations are combined with each other in each generation and form a series R with more members than the population of the previous generation. Then nondominated sorting is implemented in

series R and the entire population is classified into different ranks. To form a new generation of parents, half of the members of the R series are transferred to the next generations. The members with lower rank are preferred to those with higher rank. Then the residual population of the R series is removed from the solution process of the algorithm. After sorting the members of R series, half of these members are transferred to the next generation based on their ranking. It means that the members with lower rank are preferred to those with higher rank. When the number of transferred members is equal to population of each generation, the transfer process is stopped. Other members who are not transferred are removed from the solution process of the algorithm.

Optimization Problem

Objective Functions in Optimization Problem

Two objective functions are minimized in this study: (1) the cost of design and operation of an in situ bioremediation system (F_1) (Shieh and Peralta 2005), and (2) the SCSV in the remediation area (F_2). The equations of the objective functions are as follows:

$$\text{Minimize } F_1 = W_{F_1} \sum_{e=1}^{Nw} C_{p_e} \cdot p_e + \sum_{e=1}^{Nw} C_{IP_e} \cdot IP_e + D \left[\sum_{e=1}^{Ni} p_e \right] + E \left[\sum_{e=1}^{Ne} p_e \right] \quad (11)$$

$$W_{F_1} = [(1 + i_r)^T] / [i_r(1 + i_r)^T] \quad (12)$$

$$\text{Minimize } F_2 = \sum_{l=1}^{Nc} [C_l - C'_a]^2 \quad (13)$$

where F_1 = total present cost of design and operation of an in situ bioremediation system; W_{F_1} = factor used to convert injection/extraction costs to their present value; e = index denoting a potential injection/extraction locations; p_e = injection/extraction rate at location e (L^3T^{-1}); C_{p_e} = cost coefficient for injection (including oxygen, nutrient, and pumping costs) or extraction (including treatment and pumping operation costs) at location e (\$ per L^3T^{-1}); Nw = total number of injection and extraction wells; C_{IP_e} = injection/extraction well installation cost at location e (\$ per well); IP_e = binary variable equal to either 0 or 1 if an injection/extraction well does not exist or exists, respectively, at location e ; $D[\sum_{e=1}^{Ni} p_e]$ = oxygen and nutrient injection facility capital cost function (\$); Ni = total number of injection wells; $E[\sum_{e=1}^{Ne} p_e]$ = treatment facility capital cost function (\$); Ne = total number of extraction wells; $Nw = Ni + Ne$; i_r = discount rate; T = total duration of remediation period (year); F_2 = SCSV in all cells; l = index denoting a study area node; Nc = total number of study area nodes; C_l = contaminant concentration at location l at the end of simulation (ML^{-3}); and C'_a = clean up standard concentration (ML^{-3}).

The cost associated with an injection facility involves injecting oxygen and nutrients to the depth of contaminated groundwater, which is a function of the injection capacity. The cost of a treatment facility involves the treatment system applied on the surface to treat extracted groundwater, which is a function of the extraction capacity. Facility costs are described by integer-valued functions because the elements used in these facilities such as tubes and pumps have commercial sizes that are integer variables. Cost functions

of injection and treatment facilities are given by Eqs. (14) and (15), respectively

$$D \left[\sum_{e=1}^{N_i} p_e \right] = \begin{cases} 0 & \sum_{e=1}^{N_{if}} p_e = 0 \\ D_q & CD_{q-1} < \sum_{e=1}^{N_{if}} p_e \leq CD_q \end{cases} \quad q = 1, 2, \dots, N_{if} \quad (14)$$

$$E \left[\sum_{e=1}^{N_e} p_e \right] = \begin{cases} 0 & \sum_{e=1}^{N_{tf}} p_e = 0 \\ E_q & CE_{q-1} < \sum_{e=1}^{N_{tf}} p_e \leq CE_q \end{cases} \quad q = 1, 2, \dots, N_{tf} \quad (15)$$

where D_q = capital cost of injection facility when the total injection rate is between design injection capacity CD_{q-1} and CD_q ; N_{if} = total number of design injection capacities; q = index denoting design capacity for injection and treatment facility; E_q = capital cost of treatment facility when the total extraction rate is between design extraction capacity CE_{q-1} and CE_q ; N_{tf} = total number of design extraction capacities. The initial injection capacity CD_0 and treatment capacity CE_0 are equal to 0.

Constraints of the Optimization Problem

Constraints and boundaries must be provided depending on the characteristics of the system studied and they must be complied with by an optimal solution, if it exists. Constraint equations are

- Lower and upper bounds on injection and extraction rates;
- Lower and upper bounds on aquifer hydraulic heads at injection and extraction wells; and
- Cleanup standard concentration on monitoring wells.

These constraints are given by Eqs. (16)–(19) as follows:

$$P_{\min} \leq p_e \leq P_{\max} \quad e = 1, 2, \dots, N_w \quad (16)$$

$$HI_{\min} \leq H_e \leq HI_{\max} \quad e = 1, 2, \dots, N_i \quad (17)$$

$$HE_{\min} \leq H_e \leq HE_{\max} \quad e = 1, 2, \dots, N_e \quad (18)$$

$$C_{ow} \leq C'_{ow} \quad ow = 1, 2, \dots, N_o \quad (19)$$

where, $P_{\min}$ and $P_{\max}$ = lower and upper bounds on injection and extraction rates (L^3T^{-1}), respectively; H_e = aquifer hydraulic heads in a well at location e (L); $HI_{\min}$ and $HI_{\max}$ = lower and upper bounds on aquifer hydraulic head at injection wells (L), respectively; $HE_{\min}$ and $HE_{\max}$ = lower and upper bounds on aquifer hydraulic head at extraction wells (L), respectively; C_{ow} = contaminant concentrations on monitoring wells (ML^{-3}); C'_{ow} = cleanup standard concentration on monitoring wells (ML^{-3}); and N_o = total number of monitoring wells.

Decision Variables of the Optimization Problem

The decision variables are the independent variables that determine the value of the objective function in the optimization problem. The optimal values of the objective functions are calculated with the optimum decision variables. In the optimization problem considered in this study, the decision variables are a series of 13 numbers. These variables include injection and pumping rates. The first seven numbers of this series are the injection rates, and other remaining six numbers are the pumping rates.

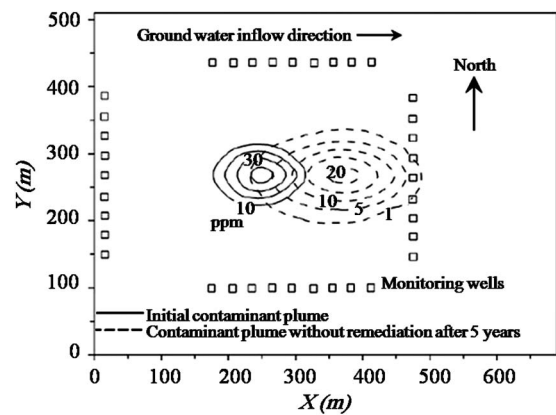


Fig. 2. Map of the case study

Case Study

A case study (introduced by Shieh and Peralta 2005) was implemented to evaluate the performance of a simulation-optimization model used for in situ bioremediation of groundwater contaminated with dissolved petroleum hydrocarbons. The considered aquifer and contaminant plume are shown in Fig. 2. The dimensions of this area are 510×690 m. This aquifer is homogeneous and its hydraulic conductivity is 6×10^{-5} m/s. The aquifer thickness is assumed constant and equal to 15 m. In the eastern and western boundaries, hydraulic head is constant and equal to 30.5 and 27.7 m, respectively. Groundwater flows from west to east and the initial hydraulic gradient equals 0.004. To the northern and southern perimeters are no-flow boundaries. Groundwater flow is at steady state. The contaminant retardation factor is assumed to equal 1.

The contaminant plume configuration after 5 years without any remediation system is illustrated in Fig. 2. It moves and expands throughout the aquifer and ultimately reaches monitoring wells downstream of the contaminated area. Natural aerobic decay reduces the total contaminant mass by 16%. An in situ bioremediation system could be installed in the contaminated area to biodegrade contaminants and prevent their spreading. For this purpose, a combination of injection and extraction wells is applied. Fig. 3 illustrates the potential locations of these wells.

Seven potential locations are assumed for injection wells specified by the letter U , which may inject oxygen and nutrients in the aquifer. The injection rates in these wells are between 0 to 1.26 L/s. The lower and upper boundaries of aquifer hydraulic heads in injection wells are 27.7 and 33.5 m, respectively. The six potential locations for extraction wells are specified by the letter E . The pumping rates in these wells are between 0 to 1.26 L/s. The lower and upper boundaries of aquifer hydraulic heads in extraction wells are respectively 24.4 and 30.5 m. Activated carbon treatment is applied for treating groundwater contaminated with dissolved petroleum hydrocarbons.

The initial concentration of oxygen in groundwater is 5 mg/L. It is 0 mg/L in the contaminated area because of (aerobic) respiration. The vertical exchange of oxygen with the unsaturated zone is assumed to be insignificant. The concentration of injected oxygen is 8 mg/L. The contaminant considered in this study is phenol. The cleanup standard concentration for phenol equals 3 mg/L.

Injection wells are embedded in the upstream zone and in the center of the contaminated plume to deliver the oxygen and nutrients for growth of microorganisms. The extraction wells are embedded in the downstream zone of the contaminated area. This

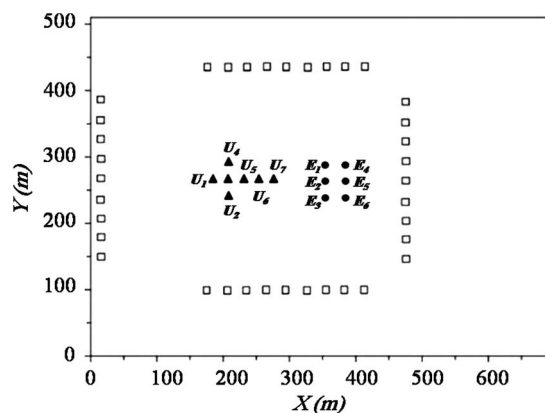


Fig. 3. Potential locations of injection (U) and extraction (E) wells

prevents the transport of residual contaminants from in situ bioremediation towards the exterior areas bordering the treatment area.

Additional monitoring wells are installed in the western, southern, and northern boundaries because the system could potentially inject excessive water. These wells are not part of the optimization. They are used to monitor the plume during a three-year remediation period. This helps ensure that unacceptable contaminant plume spreading does not occur. The maximum allowable contaminant concentration of phenol that monitoring wells can reach is 1 mg/L.

Parameters of the Simulation Model

In this study, *BIOPLUME II* was used to simulate the groundwater movement and dissolved contaminant transport. Contaminant and aquifer characteristics are required to simulate in situ bioremediation processes. This information is provided as a text input file and the simulation model reads the input data. Table 1 presents the information required for modeling the case-study problem with *BIOPLUME II*. To simplify the simulation model, several assumptions were made in this problem. These assumptions include: (1) 2D steady-state groundwater flow, (2) confined aquifer, (3) simple chemical reactions, and (4) adsorption equilibrium of the contaminant between the water and soil phases.

Cost coefficients to estimate the total cost of the bioremediation system are presented in Table 2, where it is seen that the costs of treatment facilities are linearly rates to the injection and extraction rates. Another trait about these costs is that the treatment facility costs are higher than the injection facility costs.

Results and Discussion

Results of the Single-Objective Optimization

In this part of the analysis the simulation-optimization (S-O) model was written as a single-objective problem to ensure the accuracy of this model for optimal design and operation of an in situ bioremediation system. The total cost of the project was minimized by applying the GA. The effect of changing the parameters of the GA on the optimum results was considered to evaluate the best values of these parameters for using in the optimization. After performing a sensitivity analysis, the number of populations, number of generations, and the crossover and mutation rates were selected to be 30; 20,000; 0.7; and 0.1, respectively.

Shieh and Peralta (2005) applied the GA, simulated annealing (SA), and parallel recombinatory simulated annealing (PRSA) to

Table 1. Input Parameters of the *BIOPLUME II* Model

Input parameter	Value	Units
Grid size	30 × 30	m × m
Cell number	19 × 25	—
Hydraulic conductivity	6×10^{-5}	m/s
Aquifer thickness	15	m
Hydraulic gradient	0.004	—
Longitudinal dispersivity	10	m
Transverse dispersivity	2	m
Effective porosity	0.3	—
Retardation factor	1	—
Anisotropy factor	1	—
Injected oxygen concentration	8	mg/L
Initial oxygen concentration	5	mg/L
Remediation time	3	years

Table 2. Coefficients of the Cost Objective Function

Coefficient	Value	Unit
i_r	5.50	—
C_{p_i} for injection cost	4,755	\$ per L/s-year
C_{p_e} for extraction cost	15,850	\$ per L/s-year
C_{IP_e}	12,000	\$ per well
D_q		
$D_{1.26 \text{ L/s}}$	20,000	\$
$D_{2.52 \text{ L/s}}$	24,000	\$
$D_{3.79 \text{ L/s}}$	28,000	\$
$D_{5.05 \text{ L/s}}$	32,000	\$
$D_{6.31 \text{ L/s}}$	36,000	\$
$D_{7.57 \text{ L/s}}$	40,000	\$
$D_{8.83 \text{ L/s}}$	44,000	\$
E_q		
$E_{1.26 \text{ L/s}}$	30,000	\$
$E_{2.52 \text{ L/s}}$	38,000	\$
$E_{3.79 \text{ L/s}}$	46,000	\$
$E_{5.05 \text{ L/s}}$	54,000	\$
$E_{6.31 \text{ L/s}}$	62,000	\$
$E_{7.57 \text{ L/s}}$	70,000	\$

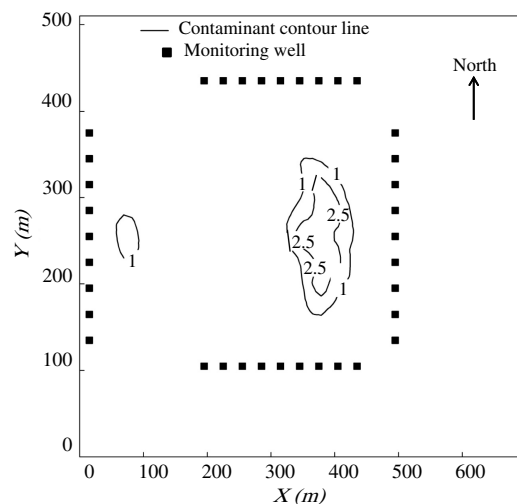
solve the problem studied in this paper. Table 3 lists the results of this study obtained by running the S-O model 10 times, and compares these with the results obtained by Shieh and Peralta (2005).

According to Table 3, the best value of the objective function reported by Shieh and Peralta (2005) was \$188,500 and this result is obtained using the PRSA approach. As can be seen in Table 3, the value of the objective function in the present study is \$187,956, which is better than result achieved with the PRSA approach. Also the total cost is \$188,282 when the number of iterations is equal to 9,943, indicating that the presented S-O model has better accuracy and performance (convergence rate) than the PRSA approach. The optimum location of wells is the same in both studies and they are selected symmetrically. Three injection wells are embedded in the center of the contaminant plume and one extraction well is embedded in the downstream zone of the contaminant plume along it is central axis. The symmetry of the initial contaminant plume is the reason of this pattern of wells. Fig. 4 illustrates the residual contaminant concentration in the aquifer after applying the optimal in situ bioremediation design. Fig. 4 shows that the residual contaminant concentration throughout the aquifer is lower than the cleanup standard (3 mg/L). The contaminant concentrations in all of the monitoring wells are less than its maximum allowable value.

Table 3. Comparison of Single-Objective Optimization Solution with Results Presented by Shieh and Peralta (2005)

Source	Optimization approach	Objective function value (\$)			Number of iterations	Selective wells
		Minimum	Average	Maximum		
Shieh and Peralta (2005)	SA	197,300	215,000	248,400	7,767	U_1, U_2, U_3, U_4, E_2
	GA	196,500	209,000	227,600	13,100	U_1, U_2, U_4, E_2
	PRSA	188,500	193,900	199,300	13,100	U_1, U_2, U_4, E_2
Present study	GA	187,956	196,252	202,294	20,000	U_1, U_2, U_4, E_2

Note: E = extraction wells; U = injection.

**Fig. 4.** Residual contaminant plume in the aquifer after impliment of optimal in situ bioremediation

Results of the Multiobjective Optimization

NSGA II is a population-based optimization method. The number of calculations of the objective functions depends on the total number of populations in each generation and on the total number of generations. Therefore, finding the best numbers of populations and generations is indispensable to the success of the optimization. These numbers were derived by sensitivity analysis in this study and equal to 30 populations and 20,000 generations.

After determining the S-O model parameters, this model was implemented using all the input information for the problem solved. The solutions of multiobjective (dual objectives, cost minimization, and SCSV) optimization are presented as a Pareto boundary that is formed by a series of optimal solutions depicted as points on the boundary. To ensure the accuracy of the obtained results from the model and the accuracy of the extracted Pareto boundary points, the problem was solved 10 times. For all Pareto combinations, an assessment criterion was used based on the Euclidean distance from an ideal point that in this case is the origin of coordinates. All Pareto points are sorted in Table 4 according to increasing Euclidean distance.

According to Table 4, the best value of the Euclidean distance equals 77,624.85 (m) and the lowest total cost in this Pareto listed in Row 1 is equal to \$200,617. Also, the lowest total cost is related to the Pareto listed in Row 6 at \$194,990.8, and the Euclidean distance of this Pareto equals 87,855.61 (m).

Fig. 5 shows the Pareto points with the best Euclidean distance and those with the lowest total cost when the residual contaminant concentrations are lower than the cleanup standard.

After merging all of the Pareto solutions and ranking these points, dominated points are removed and the remaining points

Table 4. Sorting of Pareto according to Eudidean Distance

Option number	Euclidean distance (m)	Lowest total cost (\$)
1	77,625	200,617
2	78,884	217,508
3	81,410	201,908
4	84,911	199,686
5	86,604	221,190
6	87,856	194,991
7	90,968	221,105
8	98,899	220,955
9	100,253	259,965
10	101,213	243,708

form a Pareto boundary as a final solution of the multiobjective optimization problem. The nondominated Pareto boundary is shown in Fig. 6.

This Pareto consists of a series of optimal options. Each of these options could be selected and implemented, the selection depending on the importance attached to the objective functions based on professional judgment and experience. In other words, each of these options can be selected or deselected by decision makers depending on the value of the objective functions and prevailing conditions at the existing facility. For example, the first point on the left end of a Pareto boundary detects an option that gives all the importance to the cost objective function without any weight attached to the water-quality objective function. The importance of the cost objective function is reduced and that of the quality objective function is increased by moving from left to right along the Pareto boundary. In the middle of the Pareto boundary, the objective functions have identical levels of importance. On the righthand side end of the Pareto boundary, highest importance is given to the water-quality objective function without any weight given to the cost objective function. Table 5 demonstrates the decision variables of the optimal options. The injection and extraction rates are marked with letters U and E , respectively.

According to Table 5, the largest number of injection and extraction wells was selected in Option 1. In this option, three injection and two extraction wells are selected as the optimal decision variables. One remarkable feature is that the injection wells in Option 1 are located at the center of the initial contaminant plume (according to Fig. 3). Gradually, with increasing distance from Option 1, and approaching to Option 31, the number of selected wells is reduced.

After Option 3, the selected wells for all options are injection wells. In other words, by increasing the distance from Option 1, the value of the water-quality objective function is decreased and the cost objective function is more valuable. Therefore, by moving from right to left on the Pareto boundaries, there are options that have lower costs and more SCSV than those options situated towards the right on the Pareto boundary. The number of selected wells in these options is reduced to improve the cost objective

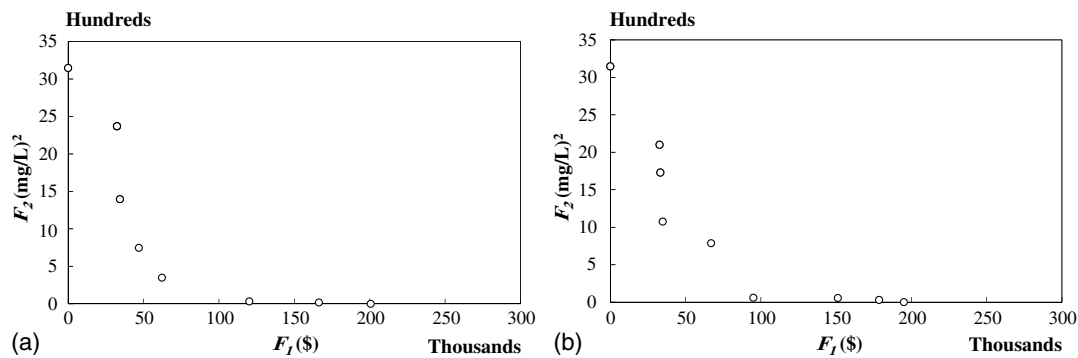


Fig. 5. Optimal Pareto: (a) with the best Euclidean distance; (b) with the lowest total cost

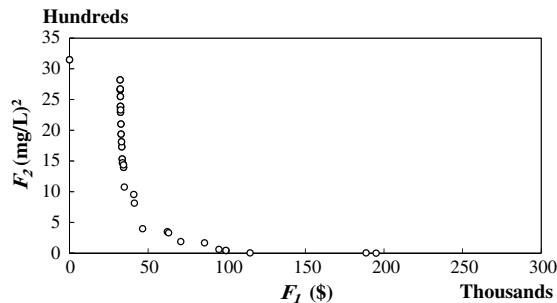


Fig. 6. Nondominated Pareto extracted from 10 optimal Pareto

function. Also, because the cost of extraction wells is higher than that of injection wells (according to Table 2), injection wells are selected as decision variables to reduce the cost of the project.

After Option 11, each option features one injection well and the injection rate is reduced. Also, the selected well location is away from the center of the contaminant plume and close to its perimeter (according to Fig. 3). In Option 31, no well is selected and no bio-remediation system is applied in this option. In this situation, a natural biodegradation process is active, and, therefore, the worst SCSV is associated with this option because a natural biodegradation is very slow process. In this study, four options of the optimal Pareto boundary were selected and the performance of

Table 5. Decision Variables of the Optimal Options

Well rates (L/s)	U1	U2	U3	U4	U5	U6	U7	E1	E2	E3	E4	E5	E6
Option 1	0.887	0.944	0	1.128	0	0	0	0.188	0.893	0	0	0	0
Option 2	0	0	1.08	0	0	0	0	0.96	0	1.094	0	0	0
Option 3	0	0	1.24	0	1.128	1.171	0.077	0	0	0	0	0	0
Option 4	0	0	1.249	0	1.209	0.284	0	0	0	0	0	0	0
Option 5	0	0	1.23	0	1.252	0.254	0	0	0	0	0	0	0
Option 6	0	0.931	0	1.192	0	0.889	0	0	0	0	0	0	0
Option 7	0	0	1.161	0	0	1.103	0.038	0	0	0	0	0	0
Option 8	0	0	0.842	0	0.911	0	0	0	0	0	0	0	0
Option 9	0	0	1.114	0	0	0	0.354	0	0	0	0	0	0
Option 10	0	0	1.121	0	0	0	0.285	0	0	0	0	0	0
Option 11	0	0	0	0	1.118	0	0	0	0	0	0	0	0
Option 12	0	0	0	0	0.713	0	0	0	0	0	0	0	0
Option 13	0	0	0	0	0	0.682	0	0	0	0	0	0	0
Option 14	0	0	0	0	0	0.217	0	0	0	0	0	0	0
Option 15	0	0	0	0	0	0	0.182	0	0	0	0	0	0
Option 16	0	0	0	0	0	0	0.18	0	0	0	0	0	0
Option 17	0	0	0	0	0	0.13	0	0	0	0	0	0	0
Option 18	0	0	0	0	0	0.115	0	0	0	0	0	0	0
Option 19	0	0	0	0	0	0.097	0	0	0	0	0	0	0
Option 20	0	0	0	0	0	0.081	0	0	0	0	0	0	0
Option 21	0	0	0	0	0	0	0.06	0	0	0	0	0	0
Option 22	0	0	0	0	0	0.056	0	0	0	0	0	0	0
Option 23	0	0	0	0	0	0	0.035	0	0	0	0	0	0
Option 24	0	0	0	0	0	0	0.032	0	0	0	0	0	0
Option 25	0	0	0	0	0	0	0.0304	0	0	0	0	0	0
Option 26	0	0	0	0	0	0	0.029	0	0	0	0	0	0
Option 27	0	0	0	0	0	0.027	0	0	0	0	0	0	0
Option 28	0	0	0	0	0	0.022	0	0	0	0	0	0	0
Option 29	0	0	0	0	0	0	0.016	0	0	0	0	0	0
Option 30	0	0	0	0	0.015	0	0	0	0	0	0	0	0
Option 31	0	0	0	0	0	0	0	0	0	0	0	0	0

Note: *E*: extraction wells; *U* = injection.

Table 6. Comparison of Four Selected Pareto Options

Considered point	Optimal value of the objective functions		Decision variables	The largest contaminant residual	Total violation of clean up standard	Rate of cost (F_1) reduction	Rate of SCSV (F_2) increases
	Cost (F_1) (\$)	SCSV (F_2) (mg/L) ²					
			(L/s)	(mg/L)	(mg/L)	(%)	(%)
Option 1	194,991	0	U_1 (0.887), U_2 (0.944), U_4 (1.128), E_1 (0.188), E_2 (0.893)	2.997	0	0	0
Option 6	94,997	59.768	U_2 (0.931), U_4 (1.192), U_7 (0.889)	7.686	26.758	51.28	1.90
Option 11	46,471	397.749	U_5 (1.118)	8.967	97.689	76.17	12.64
Option 31	0	3,147.72	—	28.379	216.650	100	100

decisions corresponding to these options was examined. The results of this comparison are listed in Table 6.

As shown in Table 6, Option 1 is the most expensive option while Option 31 does not imply any remediation cost. The remediation cost is reduced by moving from Option 1 to Option 31. The value of the water-quality objective function (defined by the SCSV) is increased by reducing the remediation cost. The third column of Table 6 displays optimal decision variables for the four chosen design options. The design Option 1 includes three injection wells and two extraction wells. This combination of wells and the injection/extraction rates corresponding to them increases the total cost of the project. Despite the high cost, the complete removal of phenol is achieved applying this option. The largest amount of residual contaminant concentration in this option is 2.997 mg/L.

In Option 6, three injection wells were selected for groundwater remediation. After implementing this option, the remediation cost is as much as 51.28% lower and the SCSVs are as much as 1.9% higher than those of Option 1. The largest residual contaminant concentration remained by implement of this option is 7.686 mg/L.

An injection well is operated in Option 11. The application of this well reduces the total cost as much as 76.17% lower than Option 1 and increases the SCSV as much as 12.64% more than Option 1. Also the largest value of residual contaminant concentration in this option is 8.967 mg/L.

In Option 31, no remediation system is applied and the contaminant is removed by natural biodegradation. In this situation, the largest residual contaminant concentration equals 28.379 mg/L. Fig. 7 illustrates the residual contaminant concentrations throughout the aquifer after applying each of these options.

According to Fig. 7, the residual contaminant concentrations throughout of aquifer are less than the cleanup standard by applying Option 1. Also the contaminant concentrations in monitoring wells at the end of the remediation time are lower than 1 mg/L, which is the standard concentration for these wells. If Option 6 is applied to remediate the aquifer, residual contaminant concentrations in the aquifer exceed the cleanup standard in many zones of the study area. Also, the contaminant plume reaches a concentration equal to 1 mg/L at the monitoring wells in the western region of the aquifer.

When Option 11 is applied for remediation of groundwater, the residual contaminant concentrations in the aquifer at the end of remediation process exceed than cleanup standard in many zones of the study site. Option 31 removes the smallest amount of contaminant and the cleanup standard is not in compliance in many zones of the aquifer. Also, no contaminant is detected in the monitoring wells at the end of remediation time.

To determine the reduction of contaminant plume during the bioremediation process, this reduction is demonstrated for Options 1 and 31 in Figs. 8 and 9, respectively. Fig. 8 illustrates the reduction

in contaminant plume in six-month intervals (0.5 years) by implementing Option 1.

As shown in Fig. 8, the contaminant plume moves downstream and gradually the concentrations of phenol were reduced. Fig. 8 shows that groundwater remediation processes reduce contaminant concentrations during three years at six-month intervals. Fig. 9 graphs the continued reduction in contaminant concentration at six-month intervals when Option 31 is applied.

As shown in Fig. 9, the contaminant plume moves downstream and gradually the concentrations of contaminant were reduced. The reduction of contaminant concentrations when Option 31 was selected is very slow because in this option, no well was operated and biodegradation is the only process active. The biodegradation is a very slow process that needed a long time to achieve meaningful results. Therefore, the residual contaminant concentrations at the end of 3 years are above the cleanup standard in many parts of the aquifer.

Sensitive Analysis of Multiobjective S-O Model

This section presents a sensitive analysis that demonstrates the sensitivity of bioremediation designs to parameters that enter in the optimization problem.

The parameters selected in this section include environmental ones and management ones. The environmental parameters include (1) hydraulic conductivity, (2) initial oxygen concentration, and (3) ratio of oxygen to hydrocarbon consumed corresponding to the type of contaminant present in the aquifer. These parameters depend on the aquifer characteristics and on the type of contaminant.

The management parameters include (1) injected oxygen concentration, and (2) remediation time. In this study, nine management scenarios are defined. Each of these scenarios involves changing one of the parameters while keeping the others constant. Table 7 demonstrates each of these scenarios, and the correspond values of the parameters.

For each of these parameters, in addition to the initial value defined in the problem, two other values were considered. One of these values is less than the initial value of the parameter and the other is larger than the initial value. After that, the optimization problem was solved based on the new values of changed parameters (lower and larger than initial value). This study considered BTEX, which is a toxic blend of fuel additives (Benzene, Toluene, Ethyl-benzene, and Xylenes), to construct the ratio of oxygen to hydrocarbon consumed.

All optimal Pareto boundaries of the multiobjective optimization for the nine different scenarios are shown in Fig. 10. In each of the graphs in Fig. 10 three Pareto boundaries are presented that represent solutions of the optimization problem based on three values assumed for each parameters (initial value, lower than initial value, and larger than initial value).

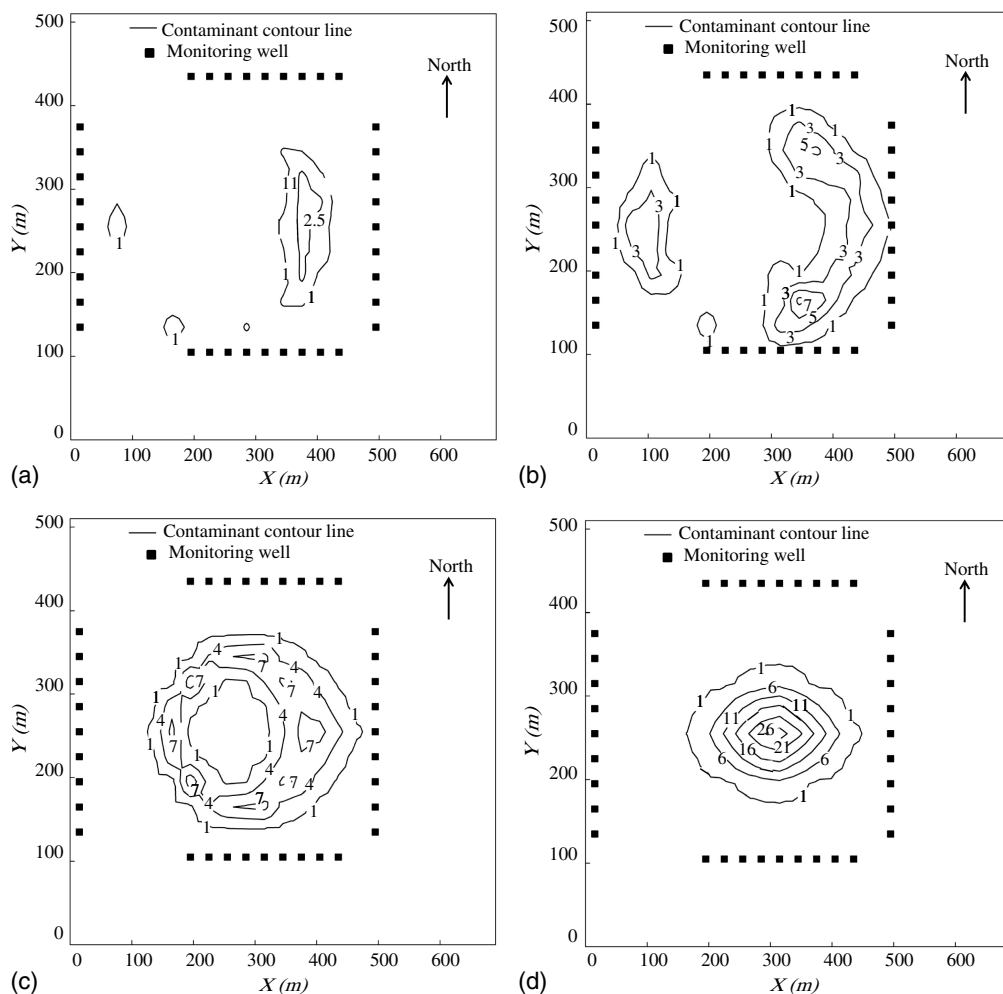


Fig. 7. Residual contaminant plume in the throughout aquifer by implementing (a) Option 1; (b) Option 6; (c) Option 11; (d) Option 31

The Pareto solutions marked with the circle points are the multiobjective optimization solutions corresponding to the initial value of each parameter. The Pareto solutions marked with the triangle points represent the multiobjective optimization solutions corresponding to a parameter value that is less than its initial value. Lastly, the Pareto solutions represented by squared points correspond to multiobjective optimization solutions corresponding to a parameter value that exceeds its initial value.

Fig. 10(a) depicts Pareto boundaries of variation of hydraulic conductivity. As can be seen in Fig. 10(a), when the aquifer hydraulic conductivity is less than its initial value and equal to 6×10^{-6} m/s, all of the Pareto points are above the initial Pareto boundary. This means that by reducing the hydraulic conductivity of the aquifer while other parameters, such as the injected oxygen concentration, are constant the remediation process is achieved with higher cost and lower performance. The reason is that by reducing the hydraulic conductivity the movement of water containing oxygen is slow and the performance of remediation process is reduced. In addition to achieving the cleanup standard, more wells must be operated. When the hydraulic conductivity is greater than its initial value and equal to 6×10^{-4} m/s, no Pareto boundary is formed and the multiobjective optimization solution is unique. This result shows that with this assumed value of hydraulic conductivity the natural biodegradation takes place and these conditions do not need any remediation system. By using this sensitivity approach and gradually varying the hydraulic conductivity,

one can determine the lowest value of the hydraulic conductivity for which bioremediation is feasible.

Fig. 10(b) portrays Pareto boundaries resulting from changes in initial oxygen concentration in the aquifer. As shown in Fig. 10(b), the three Pareto boundaries converge on the central points and a specific trend for them is not discernible. However, using the points at the two ends of these Pareto boundaries, a general trend is evident. According to the two ends of these Pareto boundaries, one can conclude that the objective value changes in a sense opposite to the changes in initial oxygen concentration. In other words, in the absence of any groundwater remediation system, increasing the initial oxygen concentration in the aquifer reduces the SCSV, and vice versa. Also, the remediation cost is reduced by increasing the initial oxygen concentration, and increased by decreasing the initial oxygen concentration.

Fig. 10(c) shows three Pareto of changes in injected oxygen concentration. As shown in Fig. 10(c) these three Pareto boundaries converge at many points and intersect each other. Therefore there is not a clear trend relating the values of the objective functions to changes in the injected oxygen concentration. However, a general trend can be seen in the two end points of the Pareto boundaries. When bioremediation is not applied, the worst SCSV in all Pareto boundaries is equal to 3,148 (mg/L)². This violation is due to residual contaminant concentration after natural biodegradation. Also, when the contaminant concentrations are less than the cleanup standard, remediation costs vary in an sense opposite to changes in the injected oxygen concentration.

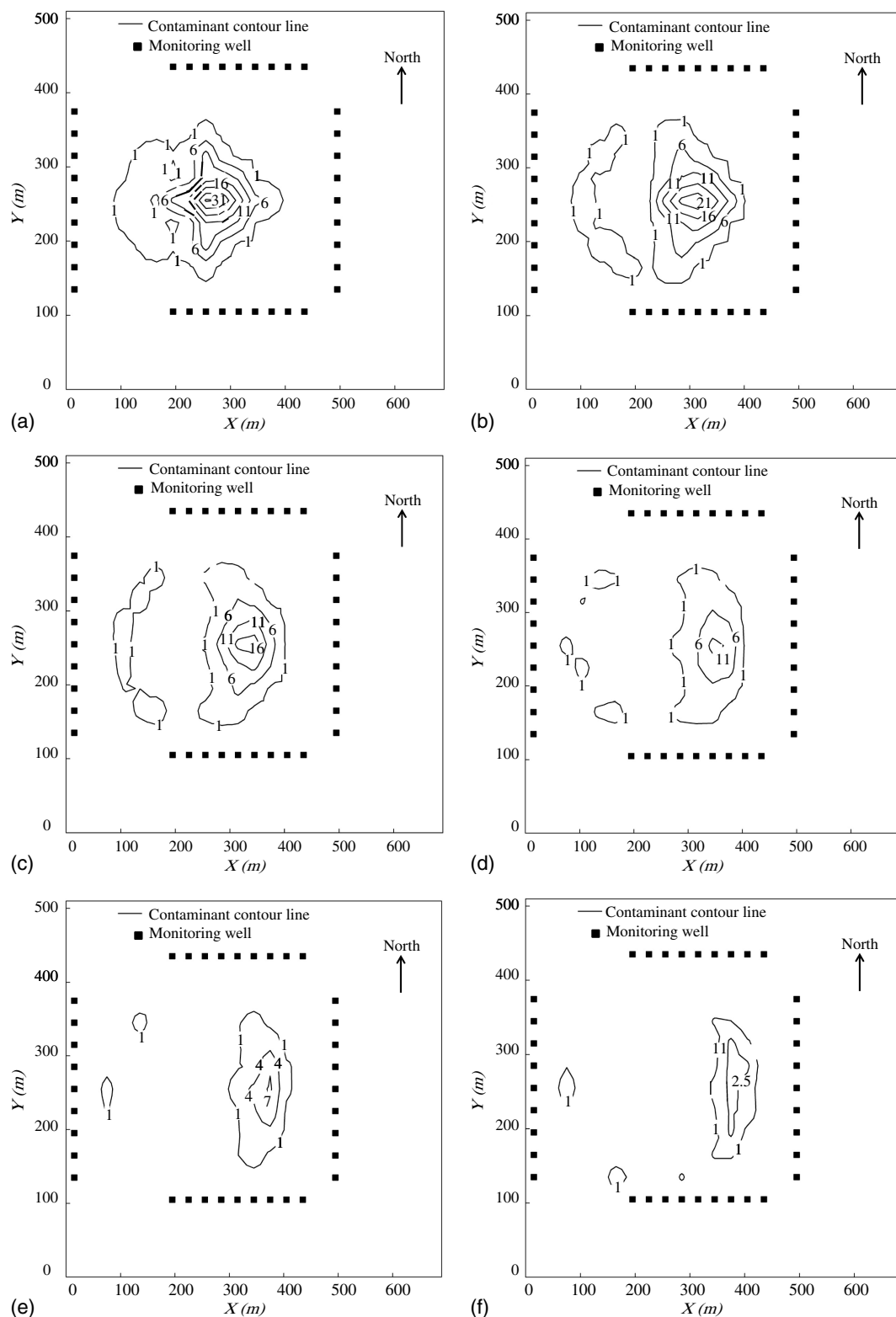


Fig. 8. Residual contaminant plume in the aquifer by implementing Option 1 after (a) 0.5 year; (b) 1 year; (c) 1.5 years; (d) 2 years; (e) 2.5 years; (f) 3 years

Fig. 10(d) shows three Pareto boundaries for changing the remediation time. As can be seen in Fig. 10(d), a general trend can be detected across the all points of these Pareto boundaries. The Pareto boundary of the shortest remediation time is above the initial Pareto, and the Pareto of the longest remediation time is under the initial Pareto. The remarkable finding is that the

objective functions vary more rapidly when the remediation time is decreased than when it is increased.

Fig. 11 portrays two Pareto boundaries corresponding to the change of the ratio of oxygen to hydrocarbon consumed corresponding to the type of contaminant present in groundwater. The Pareto boundaries indicated by the circle points represent phenol,

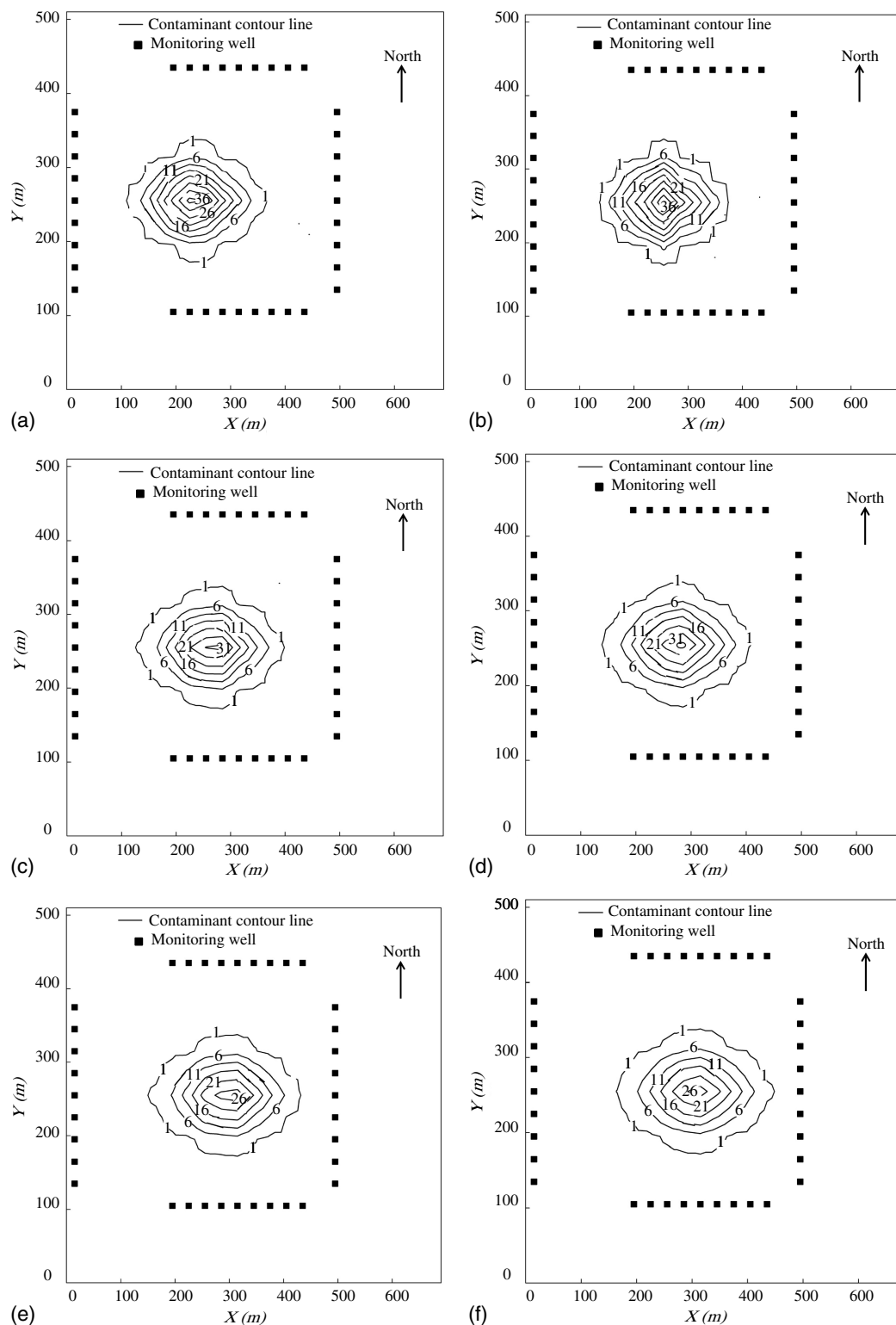


Table 7. Scenarios Considered in the Sensitivity Analysis

Number of scenario	Parameter	Symbol	Initial value	New value	Unit
1	Hydraulic conductivity	k	6×10^{-5}	6×10^{-6}	m/s
2	Hydraulic conductivity	k		6×10^{-4}	m/s
3	Initial oxygen concentration	O_{initial}	5	3	mg/L
4	Initial oxygen concentration	O_{initial}		10	mg/L
5	Injected oxygen concentration	O_{inject}	8	4	mg/L
6	Injected oxygen concentration	O_{inject}		16	mg/L
7	Remediation time	T	3	1.5	years
8	Remediation time	T		4.5	years
9	Stoichiometric coefficient	F	3	3.14	—

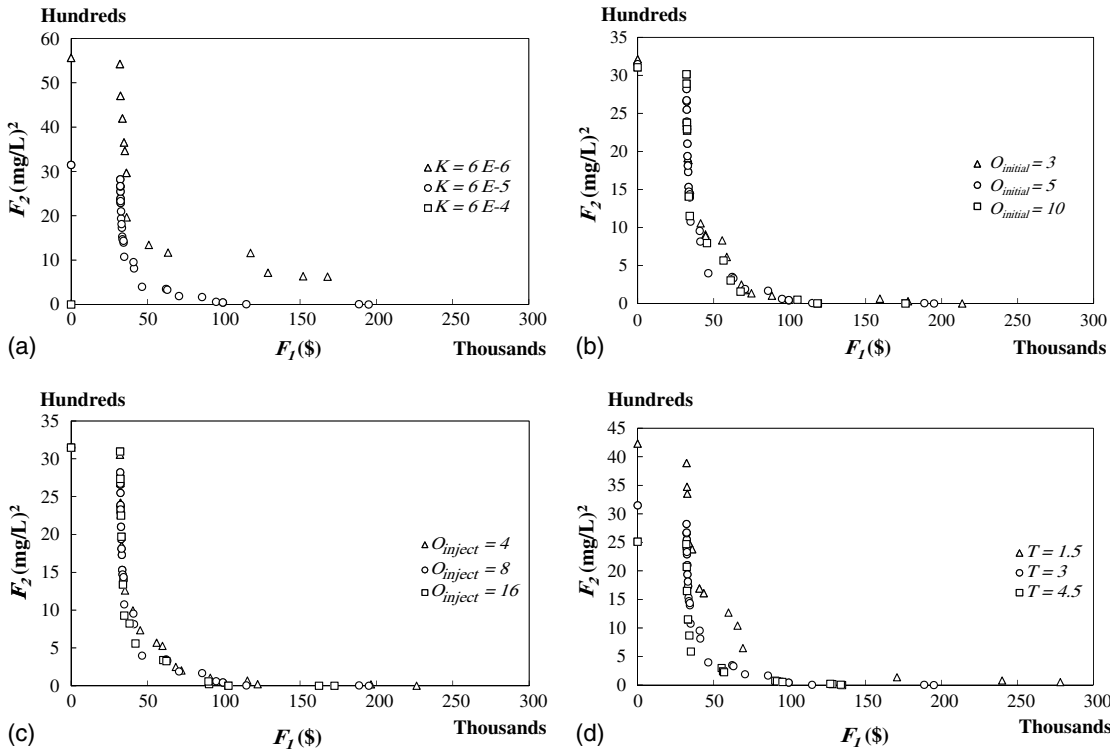


Fig. 10. Sensitivity analysis corresponding to changes of (a) hydraulic conductivity; (b) initial oxygen concentration; (c) injected oxygen concentration; (d) remediation time

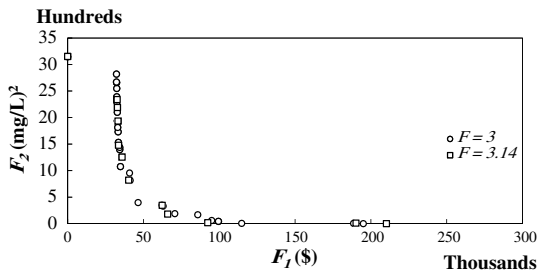


Fig. 11. Sensitive analysis for the change of the ratio of oxygen to hydrocarbon consumed

Concluding Remarks

The results obtained in this study are competitive with previous studies and indicate the good performance of the developed model. The Pareto boundary of solutions of multiobjective optimization presents a set of options for the optimal design of in situ

bioremediation. The objective functions corresponding to each of the options have different degrees of value. The two end points of the Pareto boundary of solutions represent the options with the best value for each objective function evaluated separately. The option with the highest remediation cost has the best value of the water-quality function and the option with the highest violation has the best value of the cost function. The other options are located between these two options and have different values for combinations of the two objective functions.

Sensitivity analysis of several parameters that enter the optimization problem demonstrated the effect of these parameters on the optimal solution. It was determined that the optimal solutions to the remediation problem are most sensitive to changes in the hydraulic conductivity and remediation time.

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