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Reliability-Based Multi-Objective Optimization of Groundwater Remediation

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Abstract
In-situ bioremediation of groundwater is relatively low cost and has high efficiency in remediating groundwater contaminated with petroleum hydrocarbons under suitable hydrogeologic settings. This work develops a multiobjective simulation-optimization (S-O) model for the design of an in-situ bioremediation system for petroleum-hydrocarbon contaminated groundwater. Minimizing the cost of the remediation system (installation and operation) and maximizing its reliability are the two objectives of the developed S-O model. The BIO PLUME II software simulates the remediation process and the non-dominated sorting genetic algorithm (NSGA) II optimizes remediation. The reliability objective measures the effect of uncertainty in the estimate of the initial contaminant concentration on the performance of bioremediation design, and is evaluated under five scenarios of initial contaminant concentration in an example case study illustrating this paper's methodology. The S-O model for optimal remedation calculates Pareto fronts reflecting the best tradeoff between cost and system reliability that can be obtained. Remediation managers choose remediation strategies from the calculated Pareto front that best serve their cost preferences and remediation requirements. The calculated remediation demonstrates the effectiveness of the remediation system is sensitive to the magnitude of the initial contaminant concentration.

Keywords Groundwater · In-situ bioremediation · Multi-objective optimization · Petroleum hydrocarbons · Reliability

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1 Introduction

The contamination of groundwater poses a serious threat to a resource that provides a significant portion of the freshwater used by humans worldwide. A common groundwater pollutant in oil-producing countries is petroleum hydrocarbons. Various methods have been reported to control and remediate (clean up) petroleum hydrocarbons from groundwater. Mckinney and Lin (1996) developed a nonlinear programming algorithm (NLP) and applied it to design a low-cost pump-and-treat (PAT) remediation system. Hilton and Culver (2000) developed a genetic algorithm (GA)-based method to consider the uncertainty due to hydraulic conductivity in the optimal design of a groundwater remediation system based on the PAT method. Ricciardi et al. (2007) presented an optimization method to determine the optimal design of a groundwater remediation system considering the uncertainty of the hydraulic conductivity coefficient. Ch et al. (2013) optimized the design of an in-situ bioremediation system with support vector machine (SVM) and the particle swarm optimization (PSO) algorithm. Fallah-Mehdipour (2014) developed a groundwater modeling approach based on genetic programming for the quatitative simulation of groundwater contamination. Li et al. (2015) developed an integrated simulation and optimization method for designing and managing groundwater remediation with goal planning (GP). Rezaei et al. (2017) examined the effect of uncertainty in hydraulic conductivity on the remediation of petroleum hydrocarbons. The MC Simulation (MCS) was implemented to assess the hydraulic conductivity uncertainty and BIO PLUME II was applied to simulate the in-situ bioremediation process.

The remediation of contaminated groundwater is commonly beset by high cost and long duration of the remedial operations, and by a multiplicity of processes and factors that are most successfully tackled by coupled Simulation-Optimization (S-O). S-O combines a simulation model of contaminant fate and transport with an optimization algorithm. Mantoglou and Kourakos (2007) developed a multi-objective optimization model for the optimal design of a groundwater remediation system with the PAT method under uncertainty inherent to hydraulic conductivity. Mondal et al. (2010) developed and coupled a finite element method (FEM) based groundwater-remediation simulation model with non-dominated sorting GA (NSGA II) to design an optimal remediation system. The developed model was applied in a region near Vandora in India. Singh and Chakrabarty (2011) reported an S-O model that coupled the MODFLOW 2000 groundwater model, the MT3DMS contaminant transport model, with NSGA II. The performance of the proposed S-O model was evaluated with multi-objective groundwater remediation optimization. Mutagonaker and Aldehu (2012) developed an S-O model for the optimal design of a groundwater in-situ bioremediation system. The BIO PLUME II simulated in-situ bioremediation processes and the point collocation method (PCM) solved the differential equations. The Particle Swarm Optimization (PSO) algorithm served as the optimization algorithm. Luo et al. (2012) developed a probabilistic multi-objective fast harmony search (PMOFHS) algorithm to design an optimal groundwater remediation system under uncertainty of hydraulic conductivity. Yang et al. (2013a and b) introduced a niched pareto tabu search (NPTS) algorithm and used it to optimize a PAT remediation system. The NPTS algorithm was combined with the MODFLOW and MT3DMS models in the optimal design of a groundwater remediation system in a military base in Massachusetts-USA. Yung et al. (2013) presented a fuzzy multi-objective optimization model for remediation of an oil-contaminated groundwater with the PAT method. This remediation system minimized the total pumping rate and the average post-remediation contamination density for a case study in western Canada. Kazemzadeh et al. (2014) combined the firefly algorithm (FA) optimization method with FEM for optimal designing of a PAT groundwater-remediation remediation system. The optimization model featured three objective functions with decision variables being the pumping rate and the duration of remediation. Akbarnejad et al. (2015) reported a multi-objective simulator-optimizer for designing an in-situ bioremediation system of groundwater contaminated with soluble petroleum hydrocarbons. Bio Plume II was applied for fate and transport simulation and the NSGA II solved the optimization problem. Quyang et al. (2017) presented a multi-algorithm genetically adaptive multi-objective optimization (AMALGAM) method for solving a problem of optimizating remediation of groundwater contaminated with dense non-solvent liquids.

Reliability is the probability of a system's successful performance. Hilton and Beckford (2001) evaluated the efficiency of the robust GA (RGA) algorithm introduced by Hilton and Culver (2000) for designing of a multi-objective groundwater remediation system. Ko and Lee (2008) evaluated the reliability of a PAT optimal remediation system whose sampling density in the contaminated area governed the reliability and uncertainty of the optimal remediation plan. Ghajarnia et al. (2011) developed a municipal water distribution network with the honey-bee mating optimization (HBMO) algorithm to minimize costs and maximize system reliability.

The published literature reveals an ample variety of methods for optimizing groundwater remediation. Less attention has been given to the effect that the uncertainty of key parameters of a groundwater remediation system has on its design and performance. The hydraulic conductivity, the initial concentration of the contaminant, the concentration of dissolved oxygen in groundwater, the hydrodynamic coefficients, and water-quality characteristics of the groundwater, are key parameters that affect groundwater bioremediation. Groundwater bioremedidation systems commonly assume the values of parameters even though the actual process of bioremediation may take place under conditions that vary substantially from the design assumption, which may compromise the effectiveness of groundwater remediation. This work develops a method for groundwater remediation that minimizes the cost of design and operation considering the uncertainty of the initial concentration of contaminants.

This work presents a management S-O model for the design of in-situ bioremediation system of groundwater contaminated with dissolved hydrocarbons. The objectives of the optimization problem are to minimize design and operational cost and maximize the reliability of the remediation system. Our approach evaluates the second objective of the optimization problem (maximizing reliability) with five scenarios of initial plume concentration to assess the reliability of remediation with respect to the initial contaminant concentration. The S-O model solutions produce optimal Pareto fronts that embody the optimal combinations of cost and system reliability available to system managers.

2 Simulation Model

This study implements the BIO PLUME II simulation model to simulate the process of in-situ bioremediation system of groundwater contaminated with petroleum hydrocarbons. BIO PLUME II simulates the transport of soluble hydrocarbons affected by in-situ bioremediation and prevailing oxygen availability (Konikow and Bredehoeft, 1978). Borden and Bedient (1986) reported the theory of BIO PLUME II. The growth of microorganisms and the removal of hydrocarbons and oxygen in groundwater are simulated with the modified Monod function as follows:

$$\frac{dC_{HC}}{dt} = -C_{TM}\cdot I\cdot\frac{C_{HC}}{B_{HC}+C_{HC}}\cdot\frac{C_{OX}}{B_{OX}+C_{OX}} \tag{1}$$

$$\frac{dC_{OX}}{dt} = -C_{TM}\cdot I\cdot S\cdot\frac{C_{HC}}{B_{HC}+C_{HC}}\cdot\frac{C_{OX}}{B_{OX}+C_{OX}} \tag{2}$$

$$\frac{dC_{TM}}{dt} = -C_{TM}\cdot I\cdot W\cdot\frac{C_{HC}}{B_{HC}+C_{HC}}\cdot\frac{C_{OX}}{B_{OX}+C_{OX}} + I_{OC}\cdot W\cdot C_{HC} - u\cdot C_{TM} \tag{3}$$

where C_{HC} = concentration of hydrocarbon (ML^{-3});C_{OX} = concentration of oxygen (ML^{-3}); C_{TM} = total concentration of microbes (ML^{-3}); I = maximum hydrocarbon consumption rate per unit mass of microorganisms (dimensionless); t = time (second); B_{HC} = half saturation hydrocarbon constant (dimensionless); B_{OX} = half saturation oxygen constant (dimensionless); S = stoichiometry coefficient of hydrocarbon to oxygen (dimensionless); W = coefficient of microbial efficiency (yield, dimensionless); I_{OC} = rate of first order decay of natural organic carbon (dimensionless); C_{HC} = concentration of natural organic carbon (ML^{-3}), and u = microbial rate (dimensionless).

Bear (1979) combined Eqs. (1) and (2) with the advection-dispersion equation with instantaneous and linear adsorption to yield Eqs. (4) and (5):

$$\frac{\partial C_{HC}}{\partial t} = \frac{\nabla\left(T_y\cdot\nabla C_{HC} - \upsilon_s\cdot C_{HC}\right)}{R_H} - \frac{C_{TM}\cdot I}{R_H}\cdot\frac{C_{HC}}{B_{HC}+C_{HC}}\cdot\frac{C_{OX}}{B_{OX}+C_{OX}} \tag{4}$$

$$\frac{\partial C_{OX}}{\partial t} = \frac{\nabla\left(T_y\cdot\nabla C_{OX} - \upsilon_s\cdot C_{OX}\right)}{R_H} - C_{TM}\cdot I\cdot S\cdot\frac{C_{HC}}{B_{HC}+C_{HC}}\cdot\frac{C_{OX}}{B_{OX}+C_{OX}} \tag{5}$$

where T_yTy = dispersion tensor coefficient (L^2T^{-1}); $\upsilon_s\vartheta_s$ = Darcian velocity (L^2T^{-1}); R_H R_H= hydrocarbon retardation factor (dimensionless); ∇ = the gradient operator.

BIO PLUME II assumes the exchange of microscopic living organisms between the soil surface and free solution is fast and a linear function of the concentration of microscopic living organisms. The transport of microscopic living organisms is simulated with the delay factor method described in Eqs. (6), (7), and (8) (Freeze and Cherry, 1979):

$$\frac{\partial C_{M_S}}{\partial t} = \frac{\nabla\left(T_y \times \nabla C_{M_S} - \upsilon_s \times C_{M_S}\right)}{R_M} + C_{M_S} \times I \times W \times \frac{C_{H_C}}{\left(B_{H_C}+C_{H_C}\right)} \times \frac{C_{OX}}{\left(B_{OX}+C_{OX}\right)} + \frac{I_{OC}\times W\times C_{HC}}{R_M} - u \times C_{M_S} \tag{6}$$

$$C_{M_a} = K_M \times C_{M_S} \tag{7}$$

$$C_{M_T} = C_{M_S} + C_{M_a} = (1+K_M)\times C_{M_S} = R_M \times C_{M_S} \tag{8}$$

where C_{M_s} = microbes' concentration in solution (ML^{-3}); C_{M_a} = concentration of microbes attached to soils (ML^{-3}); K_M = ratio of adsorbed microbes per microbes in solution; R_M = microbial retardation factor.

3 Non-dominated Sorting Genetic Algorithm (NSGA) II

The NSGA II is a widely used evolutionary algorithm for solving multi-objective optimization problems. The basis of this algorithm is based on the notion of "non-dominated sorting", "elitism" and optimal solution search with the genetic algorithm "GA".

4 The Genetic Algorithm (GA)

The GA was introduced by Holland (1975). This optimization method is inspired by the principles of Darwin's theory of evolution. Darwin's theory posits the fittest organisms in a variable environment have the best chance of survival. The GA begins with the generation of a random population of possible solutions, the initial population. The initial and subsequent (improved) populations consist of chromosomes (a chromosome is a possible solution). Each chromosome, in turn, is composed of a set of genes, each of which is equivalent to a decision variable of the optimization problem. The GA employs selection operators and genetic operators such as mutation and crossover operators. The selection process that improves the population of solutions from one algorithmic iteration to the next relies on the value of the fitness function (this is the objective function plus penalties for violation of constraints) corresponding to each chromosome (i.e., solution) in each generation (i.e., algorithmic iteration) and its fitness. A recent description of the GA and several other evolutionary and metaheuristic optimization algorithms can be found in Bozorg-Haddad et al. (2017).

5 Non-dominated Sorting

If a solution *i* for all objective functions is better than a solution *j*, then solution *j* is dominated by solution *i*. Furthermore, if solution *i* is better than solution *j* with respect to some objective functions, and solution *j* is better than solution *i* with respect to the others objective functions, then neither one of the two solutions is superior to the other and does not dominate the other, and these solutions are said be non-dominated with respect to each other.

Possible solutions composing a population (generation) of solutions that are not dominated by any other solutions constitute the best solutions of the population. These solutions are called first-level solutions of the non-dominate Pareto front. These first-level solutions are temporarily removed from the set of members of the current generation or population of solutions, and the best non-dominate front among the remaining solution is obtained, which constitutes the second level non-dominate front. These selection and ranking procedures continue until the current population of solutions is ranked. This method of ranking is called non-dominated sorting. The first-level non-dominate front of the population (or generation) of solutions in the last algorithmic iteration represents the best extracted (i.e., optimal) Pareto derived from the search algorithm.

6 The Process of Optimization in NSGA II

The NSGA II was introduced by Deb (2002). Each iteration of the NSGA II combines a population of parents (parent solutions) and one of children (children solutions) to generate the set R of solutions. The R set is determined by the crossover and mutation operators. The non-dominated sorting technique divides the set R, into several non-dominate fronts. The population of parent solutions in the next iteration is composed of the best members of the set R. The process of producing a new children population and combining it with the parent population to produce a new set R of solutions is repeated from one iteration to the next until achieving a convergence criterion. The technique of combining populations of parent solutions and children solutions to generate an improved generation of parents is called elitism in the the NSGA II.

7 Objective Functions

The objectives of the proposed S-O model are:

(1) Minimize the installation and operational cost of the remediation system.
(2) Maximize the reliability of the remediation system.

The decision variables are the injection and extraction rates employed in the remediation of contaminated groundwater. Five scenarios are defined to calculate the second objective. In each scenario all the model parameters are identical except for the initial contaminat concentration, which varies among the scenarios. Figure 2 shows the initial concentrations corresponding to the scenarios were set as follows:

(1) The initial contaminant concentration of Scenario 1 is 20% lower than the initial concentration implemented by Shieh and Peralta (2005).
(2) The initial contaminant concentration of Scenario 2 is 10% lower than the initial concentration implemented by Shieh and Peralta (2005).
(3) The initial contaminant concentration of Scenario 3 equals the initial concentration implemented by Shieh and Peralta (2005).
(4) The initial contaminant concentration of Scenario 4 is 10% higher than the initial concentration implemented by Shieh and Peralta (2005).
(5) The initial contaminant concentration of Scenario 5 is 20% higher than initial concentration implemented by Shieh and Peralta (2005).

Recall the first objective is minimization of the operational and design cost of the remediation system. Equations (9) and (10) are applied to calculate the cost objective, which is the same in all scenarios.

$$Minimize\,F_1 = U_C \sum_{n=1}^{Nw} C_{In} \cdot I_n + \sum_{n=1}^{Nw} C_{I'_n} \cdot I'_n + Z \cdot \left(\sum_{n=1}^{Ne} I_n \right) + Z' \cdot \left(\sum_{n=1}^{Np} I'_n \right) \tag{9}$$

$$U_C = \frac{\left[(1 + i_b)^t \right]}{\left[i_b \cdot (1 + i_b)^t \right]} \tag{10}$$

where F_1 = first objective function of the optimization problem quantifies the cost of installation and operation of the remediation system (dollars); U_C = reduction factor (converts injection/extraction costs to their present value); n = counter of potential locations of the injection and extraction wells (L^3T^{-1}); I_n = injection and extraction pumping rate of well at location n (L^3T^{-1}); C_{In} = cost coefficient for injection cost (accounts for oxygen, nutrient and pumping costs) and extraction cost (accounts for treatment and pumping operational costs) at location n ($ per L^3T^{-1}); Nw = total number of injection and extraction wells; $C_{I'n}$ = injection and extraction installation cost ar location n (dollars per well); I'_n = zero-one integer variable for injection and extraction well existence at location (1: well is installed, 0: well is not installed) n; $Z\cdot\left(\sum_{n=1}^{Ne} I_n\right)$ = the cost of oxygen and nutrient injection ($); Ne = the total number of injection wells; $Z'\cdot\left(\sum_{n=1}^{Np} I'_n\right)$ = the cost of extraction equipment ($); N_P = the total number of extraction wells; i_b = interest rate; t = total remediation time (*Year*).

The reliability index (RI_i) is defined by Eq. (11), which serves to calculate the reliability corresponding to each scenario. A reliability equal to 1 (or 0) means all the concentrations fall below (or above) the regulatory level (3 mg/L) at the end of bioremediation.

$$RI_i = 1 - \frac{\sum_{k=1}^{m} CC'_{ki}}{\sum_{k'=1}^{M} CC_{kTi}} \tag{11}$$

where RI_i = reliability index of remediation system of Scenario i; CC'_{ki} CC'_i= contaminant concentration after remediation in cells with contaminant concentration larger than 3 *mg/L*; CC_{kTi} = average contaminant concentration after remediation process; k = index for the grid cells of the simulation domain in which the contaminant concentration at the end of remediation exceeds 3 *mg/L*; k' = the counter for all the cells in the grid cells comprising the simulation domain. The second objective maximizes the reliability of the remediation system (applies to Scenarios 1 through 5):

$$Maximize:$$

$$F_2^i = RI_i \qquad i = 1, 2, 3, 4, 5 \tag{12}$$

where F_2^i = the second objective function of the optimization problem corresponding to Scenarios 1 through 5.

8 Constraints

The constraints of the optimization problem are as follows:

(1) Upper and lower limits on pumping rates in wells;
(2) Upper and lower limits on hydraulic head at injection and extraction wells;
(3) Allowable contaminant concentration at observation wells.

Equations (13) to (16) express the constraints:

Upper and lower limits on pumping rates:

$n = 1, 2, 3, \ldots, Nw I_{\min} \leq I_n \leq I_{\max}$ (13).

Upper and lower limits on hydraulic heads of injection wells:

$n = 1, 2, 3, \ldots, Ne HE_{\min} \leq H_n \leq HE_{\max}$ (14).

Upper and lower limits on hydraulic heads of extraction wells:

$n = 1, 2, 3, \ldots, Np HP_{\min} \leq H_n \leq HP_{\max}$ (15).

Upper limits on contaminant concentration:

$ow = 1, 2, \ldots, No C_{ow} \leq C'_{ow}$ (16).

where $I_{\min}$ and $I_{\max}$ = upper and lower limits on injection/extraction rates (L^3T^{-1}); H_n = well's hydraulic head located at n; $HE_{\min}$ and $HE_{\max}$ = respectively the lower and upper limit of hydraulic head in injection wells (L); $HP_{\min}$ and $HP_{\max}$ = respectively the lower and upper limit of hydraulic head in extraction wells (L); C_{ow} = contaminant concentration at observation wells (ML^{-3}); C'_{ow} = standard for contaminant concentration to be achieved by remediation at observation wells (ML^{-3}), and No = number of total observation wells.

Figure 1 illustrates the flowchart of the S-O model applied in this study. It is seen in Fig. 1 that the S-O model runs for each scenario separately. In the first step decision variables (pumping and injection rate) are generated randomly by the NSGA II, and the BIO PLUME II runs with these decision variables. The calculated state variables and the two objective functions (cost and reliability) are calculated based on the results of BIO PLUME II. The constraints and the fitness function are evaluated. The optimization algorithm stops if the stopping criteria are satisfied, and the optimal Pareto front is formed. Otherwise, the S-O

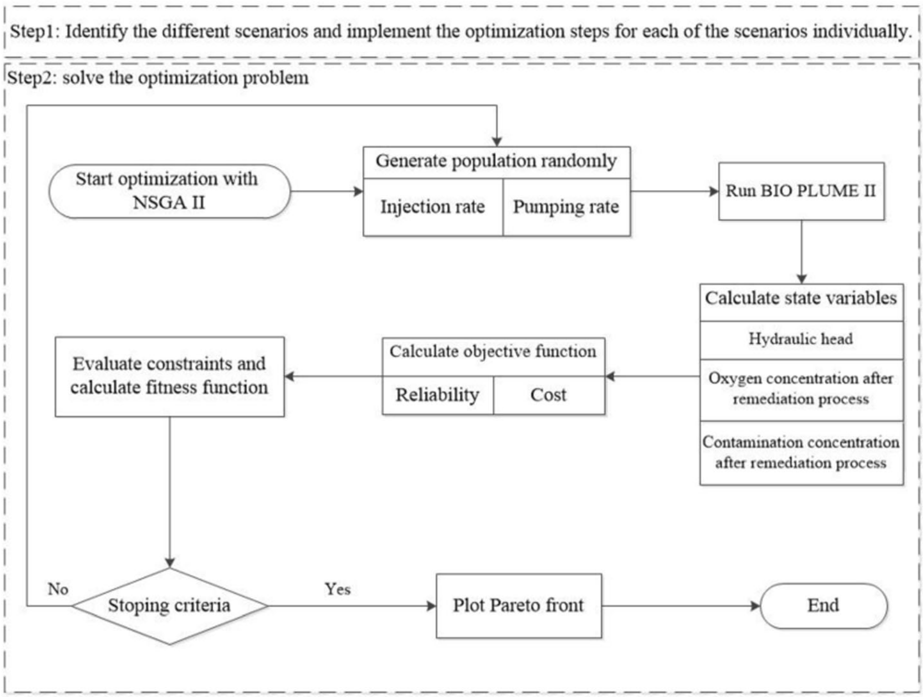


Fig. 1 Flowchart of the S-O model

model proceeds to the next iteration and the search process for optimal solutions continues until the stopping criteria is satisfied.

9 Case Study

A case study introduced by Shieh and Peralta (2005) was applied in this work to evaluate the performance of developed S-O model in optimal design of an in-situ bioremediation system. BIO PLUME II was implemented to simulate in-situ bioremediation and NSGA II was applied for optimization of remediation. The initial contaminant concentrations corresponding to the initial-concentration scenarios considered in this work are illustrated in Fig. 2.

The rectangular area of this case study has dimensions 510 m × 690 m. The aquifer is homogenous with thickness equal to 15 m. On the western and eastern boundaries, the hydraulic head is constant and equal to 30.5 m and 27.7 m, respectively. The groundwater flow direction is from west to east and the initial hydraulic gradient equals 0.004. The northern and southern boundaries are impervious (no-flow boundaries).

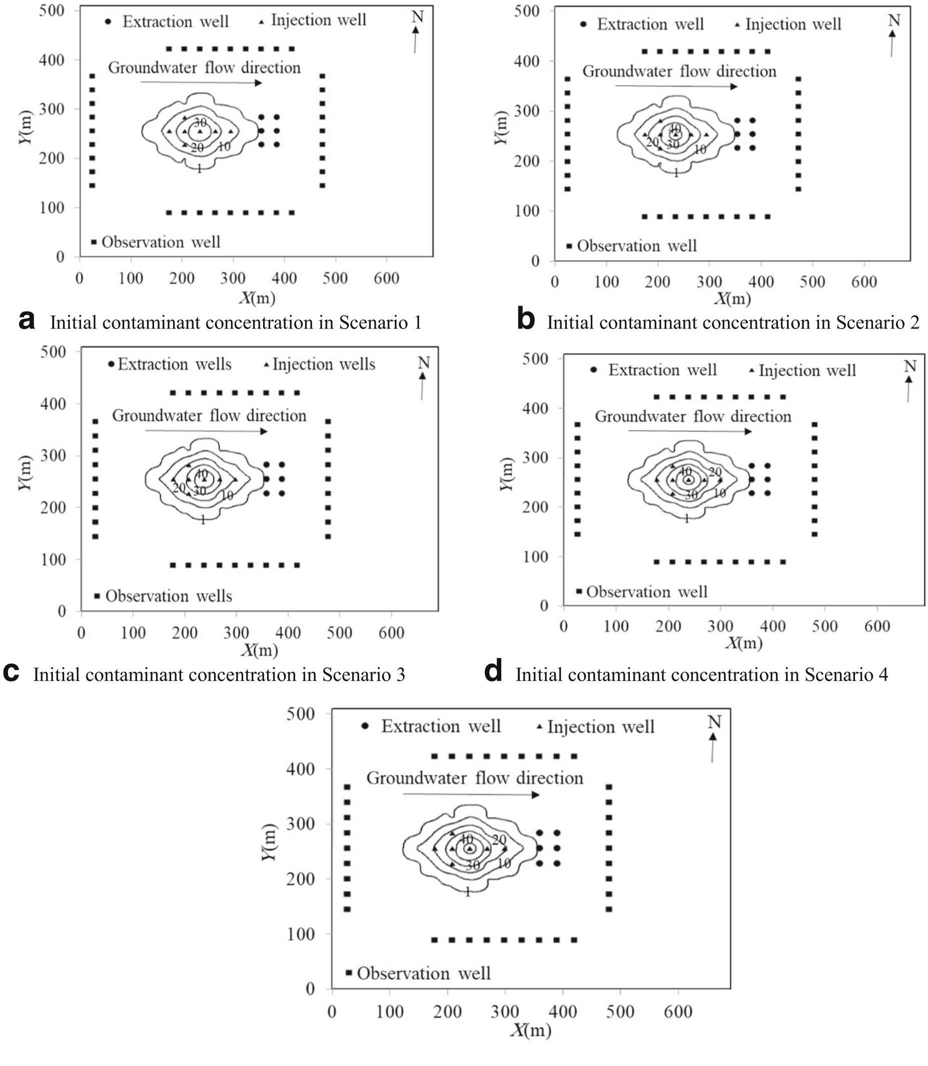
Figure 3 shows the potential locations of injection and extraction wells considered for optimization. There are seven potential locations for the injection wells (P) wherein to inject oxygen and nutrients to contaminated groundwater. There are six potential locations of extraction wells (E) with which to extract contaminated groundwater for above-ground treatment. The BIO PLUME II parameters are listed in Table 1.

10 Results and Discussion

The NSGA II parameters were estimated by sensitivity analysis, yielding optimal values of the number of populations, number of iterations, crossover factor, and mutation factor equal to 30, 1000, 0.7, and 0.2, respectively. The S-O model was run for the considered scenarios of initial concentration. The calculated optimal Pareto fronts for all scenarios are displayed in Fig. 4.

The calculated Pareto fronts are made of Pareto sets or combination of points each defining injection and pumping rates at specific wells to optimize the bioremediation objectives, which are cost minimization and reliability maximization associated with the scenarios of initial concentration. Remediation managers choose one of the Pareto sets identified by the Pareto fronts based on the priorities assigned to the remediation objectives in decision-making conditions. It is seen in Fig. 4 the installation and operational cost of the remediation system ranges between zero and $ 241,000. It is also seen in Fig. 4 the second objective of the optimization problem (maximize reliability of bioremediation) varies between zero and 100%. The Pareto fronts shown in Fig. 4 indicate generally rising reliability of remediation with increasing cost. The shapes of the Pareto fronts are influenced by the initial contaminant concentration considered by the scenarios employed in this work. The effect of initial concentration is clearly evident in Fig. 4. It is seen in Fig. 4 that for a specific cost the reliability of remediation decreases with increasing initial concentration.

Table 2 lists optimal sets of pumping (P) and extraction (E) rates obtained from the Pareto fronts associated with Scenarios 1 through 5. It is seen in Table 2 the largest number of injection and extraction wells selected for groundwater remediation system pertains to Pareto set 1 of all scenarios. Specifically, Pareto set 1 prescribes three injection wells and two extraction wells under Scenarios 1 and 2, it prescribes four injection wells and two extraction



a Initial contaminant concentration in Scenario 1

b Initial contaminant concentration in Scenario 2

c Initial contaminant concentration in Scenario 3

d Initial contaminant concentration in Scenario 4

e Initial contaminant concentration in Scenario 5

Fig. 2 Initial contaminant concentration in each scenario. The Figures show the 1, 10, 20, 30, and 40 mg/L iso-concentration lines. (A) Initial contaminant concentration in Scenario 1 (B) Initial contaminant concentration in Scenario 2 (C) Initial contaminant concentration in Scenario 3 (D) Initial contaminant concentration in Scenario 4 (E) Initial contaminant concentration in Scenario 5

wells in Scenarios 3, 4, and 5. It is noteworthy injection well E3 is selected in Pareto set 1 of all scenarios because it is located at the center of the contamination plume. The number of selected wells decreases with increasing distance from Pareto set 1, as is the case, for instance, with Pareto sets 4, 9 and 10 of Scenario 1. This means the value of the cost function and the reliability of remediation are reduced as the distance of a Pareto set increases from Pareto set 1. This confirms the previous statement that the calculated Pareto fronts display reduced remediation reliability with decreasing cost. Also, injections wells are preferable insofar as cost is concerned because their cost is lower than the cost of extraction wells. The Pareto sets with

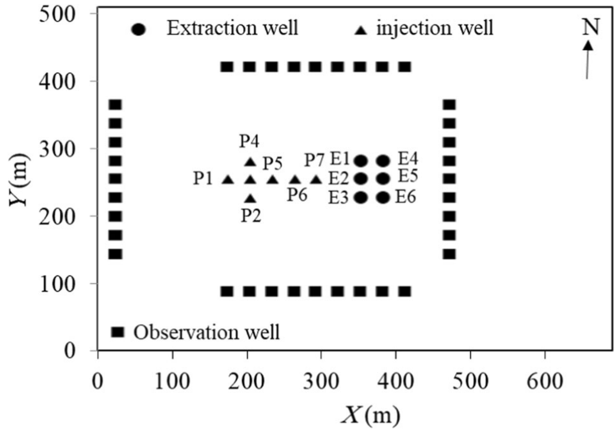


Fig. 3 Proposed locations of injection and extraction wells

high numbers (say, 8, 9, 10 whenever applicable) prescribe no extraction wells or injection wells, which means remediation proceeds naturally, albeit with minimal effectiveness as described below (Table 3).

Pareto set 1 of all scenarios achieves 100% remediation reliability with high cost. Pareto set 2 of Scenario 1 prescribes four injection wells for remediation. This choice of wells compared to Pareto set 1 reduces the cost of remediation by 36% and reduces the system's reliability by 12%. Pareto set 8 of Scenario 1 prescribes one injection well for remediation, which has a much lower costs that Pareto sets 1 and 2. The cost and reliability of Pareto set 8 would be 75% and 70% lower than the cost and reliability of Pareto set 1, respectively. The tradeoff between cost and reliability is a feature of all the Pareto fronts (see Figs. 4). For example, Pareto set 5 of Scenario 3 prescribes three injection wells and one extraction. This combination of wells reduces the cost of the project by 22% and the reliability of the system by 51% relative to Pareto set 1 of this scenario. Similarly, Pareto set 7 of Scenario 3 prescribes two injection wells, which reduces the cost by 71% and reliability by 79% relative to Pareto set 1 of this scenario.

Table 1 Input parameters to BIO PLUME II

Input parameter	Value	Unit
Grid size	30×30	–
Cell size	19×25	*m × m*
Groundwater thickness	15	*M*
Hydraulic conductivity	6×10^{-5}	*m/s*
Hydraulic gradient	0.004	–
Longitudinal dispersivity	10	*M*
Transverse dispersivity	2	*M*
Effective porosity	0.3	–
Retardation factor	1	–
Anisotropy factor	1	–
Injected concentration of oxygen	8	*Mg/L*
Initial concentration of oxygen	5	*Mg/L*
Remediation time	3	*Years*

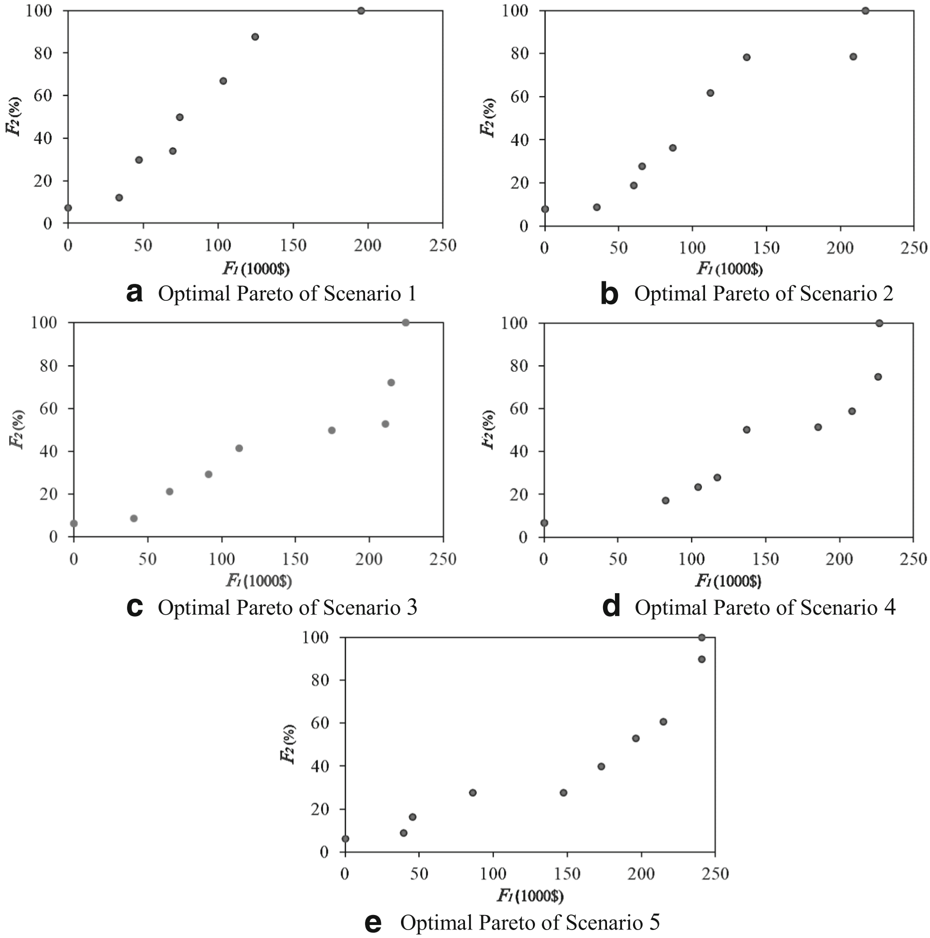


Fig. 4 Optimal Pareto for Scenarios 1 through 5. (A) Optimal Pareto of Scenario 1 (B) Optimal Pareto of Scenario 2 (C) Optimal Pareto of Scenario 3 (D) Optimal Pareto of Scenario 4 (E) Optimal Pareto of Scenario 5

Figure 5 shows the residual (that is, at the end of remediation) contaminant concentration in the aquifer in mg/L applying Pareto set 1 of Scenarios 1 through 5. It is evident in Fig. 5 that applying Pareto set 1 of Scenarios 1 through 5 produces residual contamination concentration less than three 3 mg/L, the regulatory standard. In addition, the contaminant regulatory level at observation wells is met.

Figure 6 depicts residual contaminat concentration in mg/L, corresponding to various Pareto sets and the five chosen scenarios. The pairs of Pareto set and Scenario (P, S) corresponding to Fig. 6(A), (B), (C), (D), (E), (F) are respectively (5,1), (9,1), (7,2), (4,3), (4,5), and (9,5). The Pareto sets chosen to draw Fig. 6 have the commonality of being numbered 4 or higher. Figure 6 indicates the residual concentration achieved with these Pareto sets exceeds the regulatory standard (3 mg/L). The cost of remediation system associated with these Pareto set is lower than the cost of Pareto set 1 of all scenarios, and so is the reliability of the remediation system. By

Table 2 Optimal decision variables of Scenarios 1 through 4 (Pi = pumping rate of well i; Ei = injection rate of well i, in m^3/s)

P6	P5	P4	P3	P1	P1	E7	E6	E5	E4	E3	E2	E1	Pareto sets of pumping/ injection rates	Scenario
0	0	0	0.51	0.76	0	0	0	0	0	0.84	0.57	0.62	1	1
0	0	0	0	0	0	0	1.07	0.62	1.06	0.98	0	0	2	
0	0	0	0	0	0	0	0	1.1	0.81	1.06	0.98	0	3	
0	0	0	0	0	0	0	1.09	0	0.97	0.97	0	0	4	
0	0	0	0	0	0	0	1.09	0	0	0.94	0	0	5	
0	0	0	0	0	0	0	1.09	0.58	0	0	0	0	6	
0	0	0	0	0	0	0	0	0.14	0	0	0	0	7	
0	0	0	0	0	0	0	1.16	0	0	0	0	0	8	
0	0	0	0	0	0	0	0	0	0	0	0	0	9	
0	0	0	0.8	0.57	0	0	0	0	0.65	0.76	0.57	0	1	2
0	0	0	0.8	0	0	0	0	0.89	0.66	0.8	0.57	0	2	
0	0	0	0	0	0	0.88	0.73	0.9	0	0.74	0	0	3	
0	0	0	0	0	0	0	0.78	0.92	0	0.74	0	0	4	
0	0	0	0	0	0	0	0	0.91	0	0.75	0	0	5	
0	0	0	0	0	0	0	0.71	0	0	0.66	0	0	6	
0	0	0	0	0	0	0	0	0	0	0.75	0	0	7	
0	0	0	0	0	0	0	0	0	0	0	0	0	8	
0	0	0	0	0.64	0.59	0	0	0	0.83	0.98	0.58	0.81	1	3
0	0	0	1.06	0.61	0	0	0	0	0	0.78	0.56	0.87	2	
0	0	0	1.02	0.61	0	0	0	0	0.68	0.82	0.53	0	3	
0	0	0	0	0	0	0.53	0	0.37	0.85	1.02	0	0	4	
0	0	0	1.05	0	0	0	0	0	0	0.70	0.57	0.82	5	
0	0	0	0	0	0	0	0	0.60	0.83	0.96	0	0	6	
0	0	0	0	0	0	0.49	0	0	0.80	0	0	0	7	
0	0	0	0	0	0	0	0	0	0.66	0	0	0	8	
0	0	0	0	0	0	0	0	0	0	0	0	0	9	
0	0	0	0.48	0.89	0	0	0	0.52	0	0.88	1.01	0.45	1	4
0	0	0	0.72	0.77	0	0	0	0	0	0.85	1	0.43	2	
0	0	0	0	0	0	0.84	0	0.49	0	0.9	1.08	0.47	3	
0	0	0	0.72	0.77	0.73	0	0	0	0	0.85	0	0.43	4	
0	0	0	0	0.78	0	0	0	0	0.48	0.86	0.88	0.39	5	
0	0	0	0	0	0	0	0	0.43	0	0.8	1.01	0.25	6	

Table 2 (continued)

P6	P5	P4	P3	P1	P1	E7	E6	E5	E4	E3	E2	E1	Pareto sets of pumping/ injection rates	Scenario
0	0	0	0.72	0	0.73	0	0	0	0	0.85	0	0.43	7	
0	0	0	0	0	0	0.82	0	0	0	0.89	1.02	0.45	8	
0	0	0	0	0	0	0	0	0.38	0	0.93	0	0.4	9	
0	0	0	0	0	0	0	0	0	0	0	0	0	10	

Table 3 Optimal decision variables of Scenario 5 (*Pi* = pumping rate of well *i*; *Ei* = injection rate of well *i*, in m^3/s)

P6	P5	P4	P3	P1	P1	E7	E6	E5	E4	E3	E2	E1	Pareto sets of pumping/ injection rates	Scenario
0	0	0	0	0.81	0.81	0	0	0	0.71	1.19	0.74	0.55	1	5
0	0	0	0	0.82	0.81	0	0	0	0.72	1.01	0.64	0	2	
0	0	0	0	0	0.9	0	0	0	0.77	0.98	0.75	0	3	
0	0	0	0	0.9	0.82	0	0	0	0.73	0.84	0	0	4	
0	0	0	0	0.77	0	0	0	0	0	1.08	0.8	0	5	
0	0	0	0	0	0	0.64	0	0	0	0.59	0.78	0	6	
0	0	0	0	0	0	0	0	0	0	1.04	0	0	7	
0	0	0	0	0	0	0	0	0	0	0.59	0	0	8	
0	0	0	0	0	0	0	0	0	0	0	0	0	9	

applying the high-numbered Pareto sets, such as Pareto set 9 of Scenarios 1 and 5 in Fig. 6, the effectiveness of remediation is at its lowest level, and the residual contaminant concentration exceeds the regulatory standard in most parts of the aquifer.

The results obtained from the optimized bioremediation under 5 scenarios considered in this paper illustrate that the application of the developed S-O model in a real case study yields results that reflect the effect of uncertainty in the initial concentration on the performance of in-situ bioremediation. Assuming the initial contaminant concentration in the aquifer were 10% larger than the actual contaminant concentration the reliability would be reduced between 16% and 26% from the desired target level. Furthermore, if the initial concentration of the pollutant in the aquifer were 20% larger than the actual value, the bioremediation reliability would be reduced between 24.5% and 48% from the desired target. Therefore, regulators and system managers must pay attention to the effect of the uncertainty in the initial concentration on the effectiveness of bioremediation.

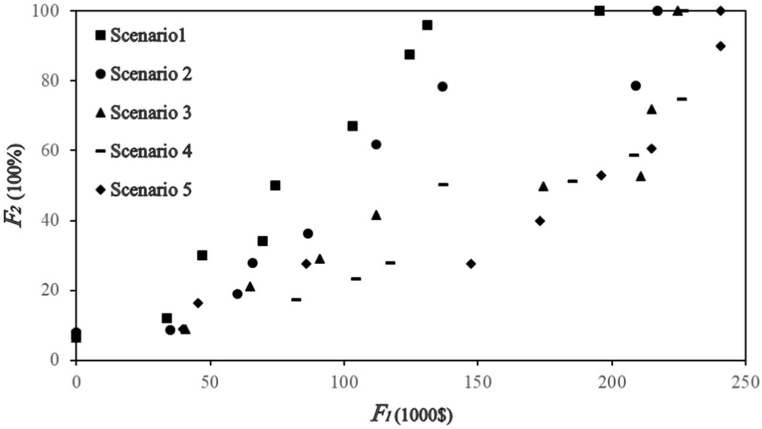


Fig. 5 Optimal Paretos of Scenarios 1 through 5. (A) Scenario 1 (B) Scenario 2 (C) Scenario (D) Scenario 4 (E) Scenario 5

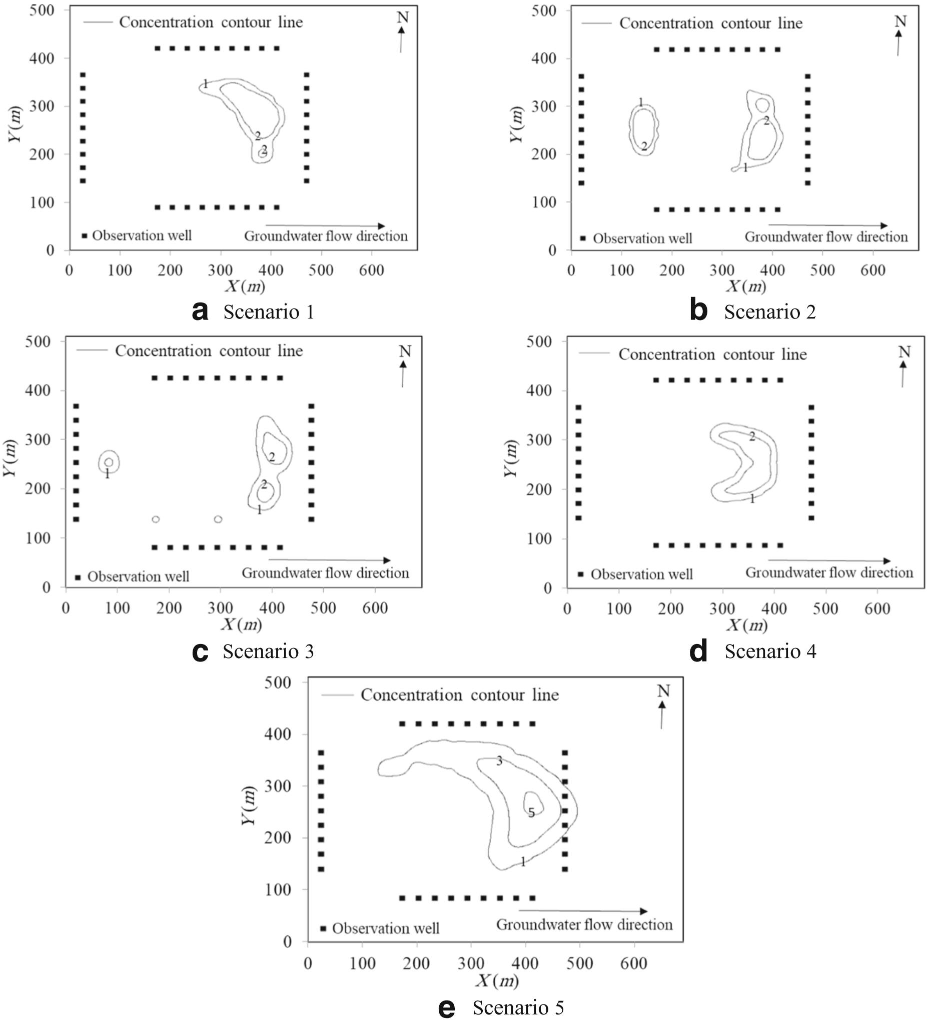


Fig. 6 Residual contaminant concentration in groundwater after bioremediation process (mg/L) corresponding to (A) Pareto set 1 of Scenario 1, (B) Pareto set 1 Scenario 2, (C) Pareto set 1 of Scenario 3, (, (D) Pareto set 1 Scenario 4, and (E) Pareto set 1 of Scenario 5

11 Concluding Remarks

A novel S-O model was applied to design an in-situ bioremediation system. The Pareto fronts derived with S-O model prescribe sets of extraction and injection rates associated with optimal combinations of costs and remediation reliability from which managers can choose based on their priorities. The optimal Pareto fronts corresponding to several scenarios of initial concentration indicate the effectiveness of remediation decreases with increasing initial contaminant concentration.

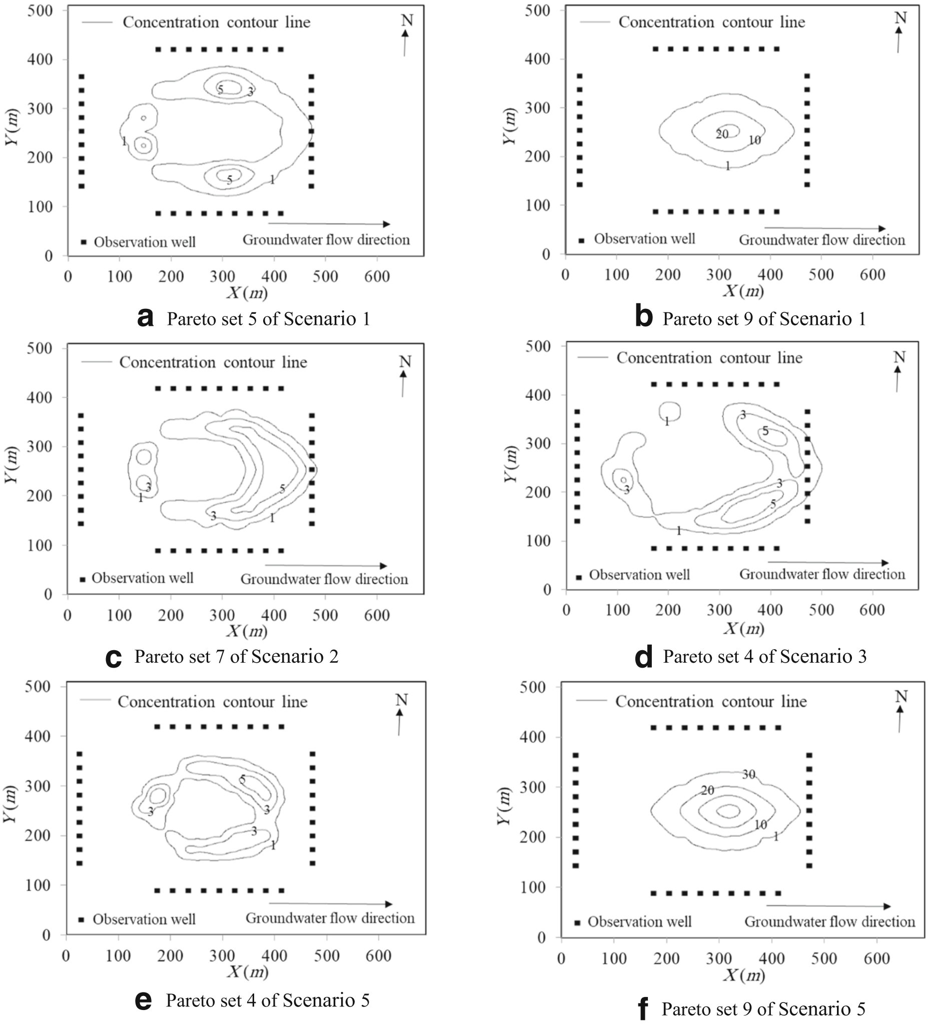


Fig. 7 Residual contaminant concentration after bioremediation process (mg/L) for (A) Pareto set 5 of Scenario 1, (B) Pareto set 9 of Scenario 1, (C) Pareto set 7 of Scenario 2, (D) Pareto set 4 of Scenario 3, (E) Pareto set 4 of Scenario 5, and (F) Pareto set 9 of Scenario 5

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Compliance with Ethical Standards

Conflict of Interests There are no conflicts of interest.

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