Multi-period aerobic groundwater bioremediation system design; ACO approach

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Abstract. The optimal groundwater bioremediation design problem is complex, nonlinear, and computationally expensive. In this paper, an improved Ant Colony Optimization (ACO) algorithm is employed for optimizing a groundwater bioremediation problem, and the BIOPLUMEII model is used to simulate aquifer hydraulics and the bioremediation process. Injection and extraction pumping rates and well locations are treated as decision variables. Optimization results show that the proposed approach performs better than the Genetic Algorithm (GA), Simulated Annealing (SA) and the hybrid SA-GA algorithm, called Parallel Recombinative Simulated Annealing (PRSA), and reduces the computational time of a number of function evaluations compared with the mentioned algorithms. Applying the optimal dynamic pumping strategy in the second stage reduces bioremediation costs by 13.3%.

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1. Introduction

A variety of technologies have been examined for restoring the quality of contaminated groundwater to achieve remedial measures such as allowed concentration of contaminant. It is usually costly to implement a remediation program due to slow contaminant-removal rates and complex hydrogeological and biochemical conditions. Therefore, finding cost effective ways for remediation programs is important. To improve remediation design, application of simulation-optimization methods has become an area of active research [1]. Previous studies have successfully developed optimization techniques to solve groundwater remediation design problems.

Examples of such optimization techniques applied to groundwater remediation design include linear programming [2], nonlinear programming [3], dynamic programming [4], simulated annealing [5], and Genetic Algorithms (GA) [6].

The solution of this complex and nonlinear problem is computationally intensive [7]. Different analytical and heuristic alternatives for a solution have been proposed to solve this problem. Heuristic methods eliminate the requirement of computing derivatives, with respect to decision variables, and are also easily coupled with simulators. One heuristic technique is the ant colony algorithm. The Ant Colony Optimization (ACO) method applied to combinatorial optimization problems was originally developed by Dorigo [8]. The formulation of this algorithm is straightforward, with no requirement for computing derivatives. The ant colony is one optimization method not applied to groundwater remediation problems.

It is the purpose of this paper to use the ant colony optimization method on a groundwater bioremediation problem to help understand when this method is likely to be computationally efficient. For testing the
performance of the ant colony algorithm, hybrid genetic algorithms from the work of Shieh and Peralta [9] are considered. In this research, well locations and pumping rates are decision variables for in situ bioremediation technology. The cost of the bioremediation process has been considered as the objective function. In the “simulation model” part, the BIOPLUMEII model has been briefly introduced, and in the “case study” part, a system design study area has been described. In the “Bioremediation design modeling”, “Model setup”, “Results and discussion” and “Conclusion” sections, an in situ bioremediation design by ACO, and summarized findings are demonstrated.

2. Materials and methods

2.1. Ant colony algorithm

Ant Colony Optimization (ACO) is a discrete meta-heuristic method that is used for solving a range of combinatorial optimization problems. The ant system was the first ACO algorithm used in the literature, but there are several variants of this. Among the available ACO algorithms, the Ant Colony System (ACS) is successfully used [10]. ACS is an efficient algorithm to solve different mathematical problems. Generally, there are few applications of ACO in water resource management [11-14].

ACO is based on the indirect communication of ants, and mediated by pheromone trails. The pheromone trails in ACO serve as distributed and numerical information, which the ants use to probabilistically construct solutions to the problem being solved and which the ants adapt during the algorithm’s execution to reflect their search experience.

In the ACO algorithm, ants are permitted to release pheromones while developing a solution or after a solution has been fully developed, or both. The amount of pheromone deposited is made proportional to the goodness of the solution an ant develops. A rapid drift of all ants towards the same part of the search space is avoided by employing the stochastic component of the choice decision policy and numerous mechanisms, such as pheromone evaporation, explorer ants and local search.

Let $\tau_{ij}(t)$ be the pheromone deposited on path $ij$ at time $t$, and $\eta_{ij}(t)$ be the heuristic value of path $ij$ at time $t$ according to the measure of the objective function. We define the transition probability from node $i$ to node $j$ at time period $t$ as follows [8]:

$$ p_{ij}(k, t) = \begin{cases} \frac{[\tau_{ij}(t)]^{\alpha} [\eta_{ij}(t)]^{\beta}}{\sum_{j' \neq j}[\tau_{ij'}(t)]^{\alpha} [\eta_{ij'}(t)]^{\beta}} & \text{if } j \in N_k(t) \\ 0 & \text{otherwise} \end{cases} $$

where $P_{ij}(k, t)$ is the probability that ant $k$ selects path $ij$ at time period $t$, $NC$ is the number of release intervals (or classes), $N_k(t)$ is the feasible neighborhood of ant $k$ when located at time period $t$, and $\alpha$ and $\beta$ are two parameters that control the relative importance of the pheromone trail and heuristic value.

Let $q$ be a random variable uniformly distributed over $[0, 1]$, and $q_0 \in [0, 1]$ be a tunable parameter. The next option, $j$, that ant $k$ chooses is [15]:

$$ j = \begin{cases} \arg \max \{[\tau_{ij}(t)]^{\alpha} \} & \text{if } q \leq q_0, t \in N_k(t) \\ J & \text{otherwise} \end{cases} $$

where $J$ is randomly selected according to the probability distribution of $P_{ij}(k, t)$ (Eq. (1)). Eqs. (1) and (2) provide a probabilistic decision policy to be used by the ants to direct their search towards the optimal regions of the search space. To simulate pheromone evaporation, the pheromone evaporation coefficient, ($\rho$), is defined which enables greater exploration of the search space and minimizes the chance of local minima upon completion of a tour by all ants. The global trail updating is done as follows:

$$ \tau_{ij}(t) = (1 - \rho) \tau_{ij}(t) + \rho \Delta \tau_{ij}(t), $$

where $0 \leq \rho \leq 1$, $(1 - \rho)$ is evaporation rate. There are several definitions for pheromone deposition on path $ij$ during time period, $t$, $\Delta \tau_{ij}(t)$. The Ant Colony System global-best (ACSgb) was chosen in this study [14] in which:

$$ \Delta \tau_{ij}(t) = \begin{cases} 1/G^{k^*_b} & \text{if } (i, j) \in \text{tour done by ant } k^*_b \\ 0 & \text{otherwise} \end{cases} $$

where $G^{k^*_b}$ is the value of the objective function for the ant with the best performance within the past total iterations.

2.2. Simulation model

In order to evaluate the aquifer system, a bioremediation model that incorporates physical, chemical, and biological processes is required. One of them is BIOPLUMEII, which has been successfully applied to field cases [16, 17]. BIOPLUMEII, previously developed by Riffat et al. [18], is a two-dimensional computer model that simulates the transport of dissolved hydrocarbons under the influence of electron acceptors (e.g. oxygen) biodegradation, and computes the variation in species concentration over time due to convection, dispersion, mixing, and biodegradation. The model is based on the United States Geological Survey (USGS) solute transport code by Konikow and Bredehoef [19]. In BIOPLUMEII, the finite difference method is used for solving hydraulic heads, and the Method Of Characteristics (MOC) is used for solving concentrations of contaminant and an electron acceptor (e.g. oxygen). It also uses instantaneous biodegradation kinetics to
simplify the problem. The contaminant and oxygen transport equations are formulated as follows [18]:

$$\frac{\partial (Ch)}{\partial t} = \frac{1}{R_c} \left[ \frac{\partial}{\partial x_i} \left( bD_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (bCV_i) \right]$$

$$- \frac{C^i W}{n_c}, \quad (5)$$

$$\frac{\partial (O_2 b)}{\partial t} = \left[ \frac{\partial}{\partial x_i} \left( bD_{ij} \frac{\partial O_2}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (bO_2 V_i) \right]$$

$$- \frac{O_2^i W}{n_c}, \quad (6)$$

where $C$ and $O_2$ are contaminant and oxygen concentrations ($M/L^3$), respectively; $C^i$ and $O_2^i$ are contaminant and oxygen concentrations in a source or sink fluid ($M/L^3$); $n_c$ is effective porosity; $b$ is aquifer saturated thickness (L); $t$ is time (T); $x_i$ and $x_j$ are Cartesian coordinates (L); $W$ is volume flux per unit area ($L/T$); $V_i$ is seepage velocity in the direction of $x_i$ ($L/T$); $R_c$ is retardation factor for the contaminant; and $D_{ij}$ is the hydrodynamic dispersion coefficient ($L^2/T$).

BIOPLOUMEII solves the solute transport equation twice; once for hydrocarbon and once for oxygen. As a result, two plumes are computed at every time step. The model assumes an instantaneous reaction between oxygen and hydrocarbon to simulate biodegradation processes. The principle of superposition is used to combine the two plumes. So, contaminant and oxygen concentration decreases at a node and are calculated from:

$$\Delta C_{RC} = O_2/F; \quad O_2 = 0 \quad \text{if} \quad C > O_2/F, \quad (7)$$

$$\Delta C_{RO_2} = CF; \quad C = 0 \quad \text{if} \quad O_2 > CF, \quad (8)$$

where $\Delta C_{RC}$ and $\Delta C_{RO_2}$ are calculated changes in contaminant and oxygen concentrations, respectively, and $F$ is the ratio of consumed oxygen to consumed contaminant.

In this research, the BIPLOUMEII is used as simulation model in the bioremediation design problem. This simulation model is coupled with an optimization method, within an overall S/O management model.

2.3. Bioremediation design problem

The example optimization problem for groundwater remediation design focuses on two systems. The first one is in situ bioremediation, which inject electron acceptors and nutrients into the contaminated groundwater, and the second one is a classic pump and treat system using granular activated carbon with air stripping technologies to treat extracted water.

Minimize cost $$\sum_{t=1}^{M^*} \left( \frac{1}{1 + i_r} \sum_{e=1}^{M^P} C^P(e)p(e, t) \right)$$

$$+ \sum_{e=1}^{M^*} C^{IP}(e)IP(e)$$

$$+ \max \left\{ D \left( \sum_{e=1}^{M^*} p(e, t) \right) \right\}_{t=1}^{M^*}$$

$$+ \max \left\{ E \left( \sum_{e=1}^{M^*} p(e, t) \right) \right\}_{t=1}^{M^*} \quad (9)$$

where cost is the total worth of the in situ bioremediation system; $1/(1 + i_r)^{yr}$ is the factor used to convert injection, extraction and treatment costs to their present value; $i_r$ is discount rate; $y_p$ is stress period duration (T); $e$ is the index of the potential injection or extraction location; $p(e, t)$ is injection or extraction rate at location $e$ for stress period $t$ ($L^3/T$); $C^P(e)$ is the cost coefficient for injection (including electron acceptor, nutrient, and pumping operation costs) or extraction (including treatment and pumping operation costs) ($\$/L^3/T$); $M^n$ is total number of stress periods; $M^P$ is total number of wells; $C^{IP}$ is well installation cost at location $e$ ($\$/well); $IP(e)$ is a zero-one integer variable for well existence at location $e$; $D(\sum_{e=1}^{M^*} p(e))$ is oxygen and nutrient injection facility capital cost, a function of total injection rate ($\$/day); $M^i$ is the total number of injection wells; $E(\sum_{e=1}^{M^*} p(e))$ is treatment facility capital cost, a function of total extraction rate ($\$/day); $M^e$ is total number of extraction wells; and $M^P = M^i + M^e$.

Facility capital cost is a discrete function of capacities. Because only specific sizes of pumps and facilities are produced, a discrete function is defined to represent the facilities capital costs. The capital cost of the injection facility is discreted as:

$$D \left( \sum_{e=1}^{M^i} p(e) \right) = 0 \quad \text{if} \quad \sum_{e=1}^{M^i} p(e) = 0,$$

$$D \left( \sum_{e=1}^{M^i} p(e) \right) = D_q \quad \text{if} \quad CD_{q-1} < \sum_{e=1}^{M^i} p(e) \leq CD_q,$$

$$q = 1, 2, ..., M^Q, \quad (10)$$

where $D_q$ is the capital cost of the injection facility when the total injection rate is between design
injection capacity $CD_{q-1}$ and $CD_q$; and $M^Q$ is the total number of alternative design injection capacities. Injection capacity $CD_0$ is 0. Eq. (11), defining the capital cost of treatment facility $E$, is analogous to Eq. (10) and obtained by substituting $E(\sum_{e=1}^{M^*} p(e,t))$ for $D(\sum_{e=1}^{M^*} p(e,t))$, $M^*$ for $M^i$, $E_q$ for $D_q$, $CE_q$ for $CD_q$, and $M^R$ for $M^Q$. $E_q$ is the treatment facility capital cost when the total extraction rate is between design treatment capacity, $CE_{q-1}$ and $CE_q$; and $M^R$ is the total number of alternative design treatment capacities. Treatment capacity $CE_0$ is 0.

$$E \left( \sum_{e=1}^{M^*} p(e) \right) = 0 \text{ if } \sum_{e=1}^{M^*} p(e) = 0,$$

$$E \left( \sum_{e=1}^{M^*} p(e) \right) = E_q \text{ if } CE_{q-1} < \sum_{e=1}^{M^*} p(e) \leq CE_q,$$

$$q = 1, 2, \ldots, M^R. \quad (11)$$

The presented objective function is discrete and non-differentiable, then it cannot be used by analytical based optimization methods. This matter is about discrete facilities and mixed integer well installation cost functions. So, ACO is mathematically capable of solving this kind of problem. Constraints can be defined as:

$$\max (p(e,t))_{e=1}^{M^*} \leq Q_{\text{max inj}}, \quad (12)$$

$$\max (p(e,t))_{e=1}^{M^*} \leq Q_{\text{max ext}}, \quad (13)$$

$$h_{\text{min}} \leq h(e,t) \leq h_{\text{max}}, \quad e = 1, \ldots, M^P, \quad (14)$$

$$C_{ij} \leq C_{tr}, \quad i = 1, \ldots, m, \quad j = 1, \ldots, n, \quad (15)$$

$$C_m \leq C_{al} \quad \forall m \in \Psi, \quad (16)$$

where $Q_{\text{max inj}}$ is the upper bound of injection rates (L$^3$/T); $Q_{\text{max ext}}$ is the upper bound of extraction rates (L$^3$/T); $h_{\text{min}}$ and $h_{\text{max}}$ are minimum and maximum allowable aquifer hydraulic heads at extraction and injection wells, respectively (L); $h(e,t)$ is aquifer hydraulic heads at well $e$ for stress period $t$ (L); $m$ and $n$ are number of cells in $x$ and $y$ direction, respectively; $C_{tr}$ is the target concentration of pollutant at the end of remediation $M/L^3$; $C_m$ is concentration at the monitoring wells $M/L^3$; $C_{al}$ is the upper bound of allowable concentration to assure prevention of pollutant migration.

2.4. Case study
The ability of the ACO algorithm was assessed in the design of a groundwater bioremediation system for a hypothetical aquifer, similar to the case studied by Shieh and Peralta [9]. The aquifer is homogeneous and isotropic. It is assumed to be contaminated with dissolved hydrocarbon. A plan view of the aquifer is shown in Figure 1, including the location of the initial contaminant plume, unmanaged plume after 5 years, and the monitoring wells. Figure 2 shows the potential remediation well sites. The potential remediation wells were grouped into two sets of locations; upgradient and downgradient. The upgradient set consists of seven potential well locations within the plume that can potentially inject water containing oxygen and nutrients. The downgradient set consists of six potential well locations that can extract contaminated groundwater. Injection and extraction rates are between 0 and 1.26 L/s.

The size of this aquifer is 510 m $\times$ 690 m, with an average depth of 15 m. In plan, a square uniform grid size of 19 $\times$ 25 is used. Two types of boundary condition, impervious or zero flux at two sides (north and south), and constant head boundaries at the other
two sides (west and east), are specified. The effective porosity of the soil is taken as 0.3. It is assumed that there is no recharge throughout the area of the aquifer. Groundwater flow simulation is steady state and the general direction of flow is from the west to the east boundary. The values of fixed head boundaries at west and east are, 30.5 and 27.7 m, respectively. Along the left and right boundaries, the contaminant concentration was set to 0 mg/L. The details of the hydraulic conductivity and initial plume are described in Table 1.

Preliminary analysis shows that the plume will reach downgradient monitoring wells after 5 years, and natural aerobic decay reduces the total contaminant mass by only 16%. In the contaminant plume area, initial oxygen concentration is zero because of aerobic biodegradation. The remainder of the aquifer area has 5 ppm oxygen concentration. The injected oxygen through the well is 8 ppm. Upper and lower bounds on the hydraulic head for the injection wells are 33.5 and 27.7 m, respectively, and the upper and lower bounds on the hydraulic head for the extraction wells are 30.5 and 24.4 m, respectively. The remediation period is 3 years and the cleanup target concentration for contaminant, $C_{tr}$, is 3 ppm for the entire study area. To avoid unacceptable plume spreading because of too much water injection, additional monitoring wells are installed at the other sides of the aquifer according to Figure 2. The maximum allowable contaminant concentration in monitoring wells, $C_{al}$, is 1 ppm. Table 2 lists the cost coefficients related to bioremediation system costs.

<table>
<thead>
<tr>
<th>Table 1. Input parameters of simulation model [9].</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Input parameters</strong></td>
</tr>
<tr>
<td>Grid size</td>
</tr>
<tr>
<td>Cell size</td>
</tr>
<tr>
<td>Hydraulic conductivity</td>
</tr>
<tr>
<td>Longitudinal dispersivity</td>
</tr>
<tr>
<td>Transverse dispersivity</td>
</tr>
<tr>
<td>Effective porosity</td>
</tr>
<tr>
<td>Retardation factor</td>
</tr>
<tr>
<td>Anisotropy factor</td>
</tr>
<tr>
<td>Injected oxygen concentration</td>
</tr>
<tr>
<td>Background oxygen concentration</td>
</tr>
<tr>
<td>Remedial time</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 2. Cost function coefficient [9].</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Coefficient</strong></td>
</tr>
<tr>
<td>$i_r$</td>
</tr>
<tr>
<td>$C_P$ for injection cost</td>
</tr>
<tr>
<td>$C_P$ for extraction cost</td>
</tr>
<tr>
<td>$C^{IP}$</td>
</tr>
<tr>
<td>$D$</td>
</tr>
<tr>
<td>$E$</td>
</tr>
</tbody>
</table>

2.5. Model setup

The proposed modeling structure has been setup for two different schemes; namely, schemes A and B. Scheme A assumes a uniform pumping rate from each well for the entire remediation horizon, whereas, in scheme B, pumping rates are permitted to vary dynamically during the remediation horizon. Scheme A has 13 different decision variables, of which 7 wells are injection and the remaining 6 are discharge wells. Due to the discrete nature of the proposed ant colony optimization algorithm, the decision space for injection and extraction wells has been discreted with uniform increments ranging from zero to 1.26 L/s. Realizing the number of decision variables of the discretization scheme, the search space will contain $7^{13}$ options, which may be classified as a medium size problem.

Scheme B assumes different injection and/or extraction rates in each period for each well. Therefore, for scheme B, there are 78 decision variables. In this case, the search space will contain $7^{78}$ different options.

In scheme A, values of 1, 0, 0.1, 1, 0.9 for the basic tunable parameters, namely, $\alpha$, $\beta$, $\rho$, $\tau_0$ and $q_0$, were set to the best values of previously reported ones [14,15,21]. Mentioned parameters for scheme B are presented in Table 3. A total number of 110 and 350 ants were used, with 60, 300 iterations for schemes A and B, respectively. To improve the quality of the solutions and reduce the chance of being trapped in local optiums, pheromone re-initiation (PRI) and Partial Path Replacement (PPR) strategies, as recommended by Hon et al. [20], and Pheromone Promotion (PP) strategies, as recommended by Jalali et al. [21], were employed.

PRI is used when the possibility of stagnation is increased (i.e., for a pre-defined number of iterations, no improvement is achieved). Pheromone concentrations in all paths are reinitialized by setting them equal to the initial value, $\tau_0$. After pheromone re-
Initiation, the search continues as normal. The PPR employed in the present algorithm is based on random displacement of some components of pairs of solutions in each iteration. To reduce computational time, in each iteration, a number of ants are chosen and parts of their solutions are randomly displaced with those of the global best from the beginning of the trail. A Pheromone Promotion (PP) mechanism is used to prevent falling in local optima. Due to pheromone deposition and evaporation, a rapid convergence syndrome or stagnation problem may prevail, if no improvement is gained after a few iterations. So, if a new solution with an improved objective value is identified, its pheromone must be promoted to the maximum existing pheromone concentration (i.e., available global best solution). If the existing pheromone concentration is very low, such an improved solution may not be desirable for the agents to follow.

3-opt is a local search procedure that is used to generate new solutions with mutations of the best ever solution produced at three decision points. In this research, the three optimization approach (3-opt), recommended by Dorigo and Gambardella [15], is used as another strategy to improve local search.

A simple flow diagram of the proposed simulation-optimization approach for the optimal design of a groundwater remediation system is depicted in Figure 3.

3. Results and discussion

3.1. Static pumping strategy (scheme A)

In all cases, the results represent the best policy found from each set of replicates. All the designs discussed meet all constraints, including the water quality con-

### Table 3. Input parameters of ant colony algorithm.

<table>
<thead>
<tr>
<th>Description</th>
<th>Scheme A</th>
<th>Scheme B</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of ants (ant)</td>
<td>110</td>
<td>350</td>
</tr>
<tr>
<td>Internal iteration (itr)</td>
<td>60</td>
<td>300</td>
</tr>
<tr>
<td>Initial pheromone (τ₀)</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Pheromone evaporation (ρ)</td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>Control parameter (α)</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Control parameter (β)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Tunable parameter (q₀)</td>
<td>0.8</td>
<td>0.9</td>
</tr>
</tbody>
</table>

### Table 4. Optimal system costs for Scheme A and B.

<table>
<thead>
<tr>
<th>Formulation</th>
<th>Mean The best</th>
<th>Mean The worst</th>
<th>S.D.</th>
<th>C. V.</th>
<th>Number of model runs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scheme A</td>
<td>191.4</td>
<td>185.9</td>
<td>200.2</td>
<td>4.8</td>
<td>0.02</td>
</tr>
<tr>
<td>Scheme B</td>
<td>164.8</td>
<td>161.2</td>
<td>170.1</td>
<td>2.5</td>
<td>0.02</td>
</tr>
</tbody>
</table>

![Figure 3. ACS algorithm for groundwater bioremediation system.](#)
Table 5. Optimal system costs of scheme A for ACO, SA, GA and PRSA (20 runs for each model).

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Well installation cost ($)</th>
<th>Injection cost ($)</th>
<th>Extraction and treatment cost ($)</th>
<th>Injection facility capital cost ($)</th>
<th>Treatment facility capital cost ($)</th>
<th>Number of simulations call</th>
<th>System cost ($)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SA [9]</td>
<td>60,000</td>
<td>36,300</td>
<td>43,100</td>
<td>28,000</td>
<td>30,000</td>
<td>7,767</td>
<td>197,300</td>
</tr>
<tr>
<td>GA [9]</td>
<td>48,000</td>
<td>38,100</td>
<td>52,400</td>
<td>28,000</td>
<td>30,000</td>
<td>13,100</td>
<td>196,500</td>
</tr>
<tr>
<td>PRSA [9]</td>
<td>48,000</td>
<td>37,600</td>
<td>44,900</td>
<td>28,000</td>
<td>30,000</td>
<td>13,300</td>
<td>188,500</td>
</tr>
<tr>
<td>ACO</td>
<td>48,000</td>
<td>36,300</td>
<td>43,600</td>
<td>28,000</td>
<td>30,000</td>
<td>6,000</td>
<td>185,500</td>
</tr>
</tbody>
</table>

In Shieh and Peralta [9], the aforementioned problem was studied by Simulated Annealing (SA), Genetic Algorithm (GA) and Parallel Recombinative Simulated Annealing (PRSA). According to Table 5, among the four optimization algorithms, ACO has the best solution, with a minimum cost of $185,900. The minimum cost resulted by the PRSA algorithm for constant pumping was $188,500. In order to achieve this solution, PRSA called the simulator (BIOLMEII), 13,300 times, while, in our approach, to achieve a minimum cost of $185,900, the ACO algorithm called the simulator 6,600 times. The ACO best solution quality is 1.38% better than the PRSA algorithm, with almost 50% reduction in the number of function evaluations (i.e. simulation calls). Results presented in Table 5 show that, for this problem, the proposed simulation-optimization scheme with the ACO algorithm performs slightly better than all the other 3 algorithms. In fact, with approximately 78%, 45% and 45% of the number of function evaluations of SA, GA and PRSA, the proposed approach resulted in slightly smaller cost, respectively.

This outcome shows the phenomenal capability of ACO algorithm in cutting calculation cost in comparison to SA, GA and PRSA algorithms.

3.2. Dynamic pumping strategy (scheme B)

In the second part of this study, the aquifer remediation horizon has been divided into multiple management intervals. The three-year remediation period is divided into 6, half-year pumping intervals. The pumping discharges can vary from interval to interval. Shieh and Peralta [9] applied varying pumping approaches using the previous selected wells (scheme A, outputs U1, U2, U4 and E2). As mentioned earlier, there are 78 decision variables for 13 wells, with 7 states as decision variables. As seen, the number of decision variables in scheme B is more than scheme A, which is 13, and this problem would be computationally more complicated and time consuming. Table 6 shows the results and cost of the optimum solution. Comparing to the constant pumping strategy, only the costs associated with injections and discharges are decreased.

The varying pumping strategy was modeled by

Figure 4. System cost versus number of model internal iterations for the best solutions.

Figure 5. Injection and extraction values for the best solution of scheme A.

less than the cost of extraction and treatment from one well. In addition, the set up cost of extraction and treatment facilities is $30,000 and higher than that of the injection facilities, $28,000, which confirms the outcome of the model in using more injection wells. Wells, identified as U2 and U4, are injected with their near maximum capacity, and well U1, which is located on the symmetry line of the study area, is being operated at near half capacity of the two other injection wells (Figure 5). The operation of injection wells, especially U1, possibly makes the problem infeasible. In some cases, where the observed concentrations in the west control wells (Figure 1) would be higher than the allowed concentration (1 ppm), the solution would be infeasible.
Table 6. Optimal system costs of scheme B for ACO and PRSA (10 runs for each formulation).

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Well installation cost ($)</th>
<th>Injection cost ($)</th>
<th>Extraction and treatment cost ($)</th>
<th>Injection facility capital cost ($)</th>
<th>Treatment facility capital cost ($)</th>
<th>Number of simulations call</th>
<th>System cost ($)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACO</td>
<td>48,000</td>
<td>24,400</td>
<td>30,800</td>
<td>28,000</td>
<td>30,000</td>
<td>105,000</td>
<td>161,200</td>
</tr>
<tr>
<td>PRSA [9]</td>
<td>48,000</td>
<td>25,800</td>
<td>31,500</td>
<td>28,000</td>
<td>30,000</td>
<td>NA*</td>
<td>163,300</td>
</tr>
</tbody>
</table>

* Not assigned.

Table 7. Injection and extraction rates of the best solutions of schemes A and B.

<table>
<thead>
<tr>
<th>Wells</th>
<th>Injection rates (lit/sec)</th>
<th>Extraction rates (lit/sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>U1</td>
<td>U2</td>
</tr>
<tr>
<td>Scheme A</td>
<td>One period</td>
<td>0.63</td>
</tr>
<tr>
<td>Period 1</td>
<td>0.12</td>
<td>1.26</td>
</tr>
<tr>
<td>Period 2</td>
<td>0.12</td>
<td>1.26</td>
</tr>
<tr>
<td>Period 3</td>
<td>0</td>
<td>1.26</td>
</tr>
<tr>
<td>Period 4</td>
<td>0</td>
<td>0.84</td>
</tr>
<tr>
<td>Period 5</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Period 6</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Shieh and Peralta [9] using the PRSA optimization algorithm, resulting in a minimum cost of $163,300. The authors indicate they have used a population size of 200, instead of 100, in the constant pumping problem. However, they did not mention the number of function evaluations or BIOPLUMEII calls. Since the problem is more complicated than the previous one, for PRSA formulation, the number of simulation calls greatly exceeds that of the static case (i.e., 13,300).

Results of the proposed scheme selects three injection wells, U1, U2, U4, and one extraction well, E2, as the optimum decision. According to Table 6, the minimum cost for the selected solution is $161,200, which is slightly (1.3%) better than the PRSA outcome. The reported near optimum solution was achieved with 105,000 function evaluations (i.e., simulation calls). The convergence behavior of the proposed ACO algorithm for the best solution of scheme B is illustrated in Figure 4.

The minimum cost obtained in the dynamic pumping strategy (scheme B) is 13.3% better than the static pumping (scheme A). In various stages of the remediation process, operation discharges vary by contamination concentration changes (Figure 6). According to Table 7, injection wells are super active during the first 4 operational intervals (first two years), in which wells U2 and U4 should be used with almost full capacity. In addition, during the last year of operation, the discharge rate of injection wells is zero. It shows that during the last two periods, contamination has moved downstream, and the injection process at upstream is no longer effective. So, in line with this movement, the optimization algorithm shows zero pumping for upstream injection wells. On the other hand, according to the results, the discharge value of well E2 during the first 2 periods is zero, which indicates that discharge wells, unlike injection wells, have no contribution during the first two periods. The far distance of the contamination plume from the downstream monitoring wells during the early periods of remediation is the reason for the inactiveness of extraction wells during the mentioned periods. By migration of contamination to the downstream, extraction wells begin their contribution, and, as it gets closer to the last operational periods, the discharge rates of those wells increase, in such a way that they reach maximum capacity during the last two periods. Figure 7 shows the final contamination plume after 6 operational periods (3 years).
4. Conclusion

In this research, an improved ant colony optimization model has been employed to optimize the in situ bioremediation design system. The model is coupled with a simulator called BIOPLUME II. Decision variables in the simulation/optimization model are the pumping values of injection and extraction wells, and the location of wells. The objective function is minimization of total system cost. Reduction of contaminant to the cleanup standard is a target in this problem. PP, PRI, PPR and 3-opt mechanisms have been employed to improve the convergence and performance of ACO algorithm, so called ACS$_{3b}$-PP-PRI-PPR-3opt.

ACS$_{3b}$-PP-PRI-PPR-3opt was compared with GA, SA and PRSA in scheme A and with PRSA in scheme B. The scheme A problem has been solved with steady, and scheme B with time varying, pumping strategies. The number of simulations in the ACO is less than the other mentioned algorithms in both schemes. Also, the quality of solutions in ACO is better too.

Results of this research show the ability of the proposed ACO algorithm in the computationally expensive problem of groundwater bioremediation system design, and show that it can be used as a method for enabling the solution of larger-scale groundwater remediation design problems.

Nomenclature

\[ \tau_{ij}(t) \] Total pheromone deposited on path \( ij \) at time \( t \)
\[ \eta_{ij}(t) \] Heuristic value of path \( ij \) at time \( t \)
\[ N_{k}(t) \] Feasible neighborhood of ant \( k \) when located at time period \( t \)
\[ NC \] Number release intervals (or classes)

\[ \alpha \] Control parameter of pheromone trail
\[ \beta \] Control parameter of heuristic value
\[ q \] Random variable uniformly distributed over [0, 1]
\[ q_0 \] Tunable parameter \( \in [0, 1] \)
\[ \rho \] Pheromone evaporation coefficient
\[ \tau_0 \] Initial pheromone value
\[ G_0^{a,b} \] Value of the objective function for the ant with the best performance within the past total iterations
\[ C \text{ and } O_2 \] Contaminant and oxygen concentration in aquifer
\[ C^i \text{ and } O^i_{2x} \] Contaminant and oxygen concentration in a source or sink fluid
\[ n_e \] Effective porosity
\[ b \] Aquifer saturated thickness
\[ t \] Time
\[ x_i \text{ and } x_j \] Cartesian coordinates
\[ W \] Volume flux per unit area
\[ V_i \] Seepage velocity in the direction of \( x_i \)
\[ R_e \] Retardation factor
\[ D_{ij} \] Hydrodynamic dispersion coefficient
\[ \Delta C_{RC}, \Delta C_{RO} \] Change in contaminant and oxygen concentrations
\[ F \] Ratio of consumed oxygen to consumed contaminant
\[ i_r \] Discount rate
\[ y_p \] Stress period duration
\[ e \] Index of potential injection or extraction location
\[ p(e, t) \] Injection or extraction rate at location \( e \) for stress period \( t \)
\[ C_p(e) \] Cost coefficient for injection or extraction
\[ M^n \] Total number of stress periods
\[ M^P \] Total number of wells
\[ C^{IP} \] Well installation cost at location \( e \)
\[ IP(e) \] Zero-one integer variable for well existence at location \( e \)
\[ M^i \] Total number of injection wells
\[ M^e \] Total number of extraction wells
\[ D_q, E_q \] Capital cost of injection and extraction facilities at different level
\[ CD_q, CE_q \] Design injection and extraction capacity at level \( q \)
\[ M^Q \] Total number of alternative design injection capacities
\[ q_{\text{max inj}} \] Upper bound of injection rates
\[ q_{\text{max ext}} \] Upper bound of extraction rates
\( h_{\min}, h_{\max} \)  
Minimum and maximum allowable aquifer hydraulic heads at wells

\( m, n \)  
Number of cells in \( x \) and \( y \) directions

\( C_{tr} \)  
Target concentration of pollutant at the end of remediation

\( C_m \)  
Concentration at the monitoring wells

\( C_{al} \)  
Upper bound of allowable concentration

\( \Psi \)  
Set of monitoring wells

References


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