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OPTIMAL SYSTEM DESIGN OF IN-SITU BIOREMEDIATION USING PARALLEL RECOMBINATIVE SIMULATED ANNEALING

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ABSTRACT

We present a simulation/optimization model combining optimization with BIOPLUME II simulation for optimizing in-situ bioremediation system design. In-situ bioremediation of contaminated groundwater has become widely accepted because of its cost-effective ability to achieve satisfactory cleanup. We use parallel recombinative simulated annealing to search for an optimal design and apply the BIOPLUME II model to simulate aquifer hydraulics and bioremediation. Parallel recombinative simulated annealing is a general-purpose optimization approach that has the good convergence of simulated annealing and the efficient parallelization of a genetic algorithm. This is the first time that parallel recombinative simulated annealing has been applied to groundwater management. The design goal of the in-situ bioremediation system is to minimize system installation and operation cost. System design decision variables are pumping well locations and pumping rates. The problem formulation is mixed-integer and nonlinear. The system design must satisfy constraints on pumping rates, hydraulic heads, contaminant concentration at the plume source and at downstream monitoring wells. For the posed problem, the parallel recombinative simulated annealing obtains an optimal solution that minimizes system cost, reduces contaminant concentration and prevents plume migration.

INTRODUCTION

In-situ bioremediation of contaminated groundwater has become widely accepted because of its cost-effective ability to achieve satisfactory cleanup. Major advantages of in-situ bioremediation include lower capital cost and permanent elimination of contaminants (Cookson, 1995). An in-situ bioremediation system consists of subsurface water delivery systems (injection wells or trenches) and extraction wells. The recharge water provides nutrients and terminal electron acceptors to stimulate microbial growth. These microorganisms transform contaminants to less harmful

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chemicals or mineral end products, such as carbon dioxide and water. The most common electron acceptor used for in-situ bioremediation is oxygen. Downgradient wells extract contaminated groundwater to contain the plume and to enhance movement of electron acceptors and nutrients. Contaminated groundwater from the extraction wells is treated by air stripping or activated carbon. Monitoring wells even further downgradient are used to verify plume containment.

This study involves optimizing in-situ bioremediation system design. Design can be enhanced by combining simulation models with optimization techniques. Design elements include well locations, pumping rates (as continuous variables), injected oxygen concentrations, and maximum contaminant levels. We use the BIOPLUME II model (Rifai et al., 1987) to simulate aquifer hydraulics and remediation response. We use parallel recombinative simulated annealing (PRSA) with BIOPLUME II to achieve optimization with simulation.

METHODOLOGY

Simulated Annealing and Genetic Algorithms

Simulated annealing (SA) is an algorithmic approach for combinatorial optimization problems. It was first introduced by Kirkpatrick et al. (1983). Convergence of simulated annealing algorithm to globally optimal solutions has been proven using homogeneous Markov chain and inhomogeneous Markov chain theory (Hajek, 1988; Romeo and Sangiovanni-Vincentelli, 1991). SA has been successfully applied to groundwater remediation problems (Dougherty and Marryott, 1991; Marryott, 1996; Rizzo and Dougherty, 1996). Another widely used optimization technique is genetic algorithms (GAs). The study of genetic algorithms (GAs) has been well documented by many researchers (Holland, 1975; Goldberg, 1989; Davis, 1991; Michalewicz, 1992; Mitchell, 1996; Bäck, 1996). GAs also have been applied to many water resources management problems such as pipe network (Simpson et al., 1994; Dandy et al., 1996), groundwater remediation (Ritzel et al., 1994; McKinney and Lin, 1994) and groundwater monitoring (Cieniawski et al., 1995). GAs are naturally parallel and can be easily run on networks or parallel computers. They iterate a entire population using crossover, mutation and selection operators. GAs have no formal proof of convergence and no good control of convergence. On the other hand, SA can be proven to converge to global optimal solutions. The proof mainly depends on the annealing schedule. By slowly decreasing an annealing parameter (commonly termed temperature), SA can use more iterations to control the convergence to optimality. SA can be viewed as a sequence of homogeneous Markov chains. This makes it difficult to parallelize simulated annealing to accelerate convergence.

Recently, researchers have investigated hybrid genetic annealing algorithms (GAAs) approaches that combine desirable attributes of GA and SA methods (Sirag and Weisser, 1987; Brown et al., 1989; Goldberg, 1990; Boseniuk and Ebeling, 1991; Lin et al., 1993; Mahfoud and Goldberg, 1995; Yong et al., 1995; Varanelli and Cohoon, 1995). The result should be a general-purpose optimization algorithm that has the good convergence control of SA and the efficient parallelization of GAs

Parallel Recombinative Simulated Annealing

In this study, we choose parallel recombinative simulated annealing (PRSA) for optimizing system design of in-situ bioremediation. Mahfound and Goldberg (1995) presented the PRSA algorithm and proved its convergence. The PRSA algorithm is an effective combination of simulated annealing and genetic algorithms. The implementation of PRSA is given in Figure 1.

```
initialize T(0);
initialize P(0) = { X1(0), X2(0), ..... XN(0) } ;
evaluate C(0) = cost function(P(0));
k , n = 0;
while (stooping criterion is not satisfied)
{
  for i = 1 to G
  { for j = 1 to N/2
    { select two parents without replacement from P(k);
      generate two children using crossover and mutation operators;
      evaluate Cchild = cost function(Xchild);
      Boltzmann trials between parents and children;
      if ( random(0,1) < 1/[1+exp((Cparent-Cchild)/T(n)] )
        select Xparent;
      else
        select Xchild;
    }
    P(k+1) = { X1(k+1), X2(k+1), ....., XN(k+1) };
    k = k +1;
  }
  T(n+1)= temperature update function(T(n));
  n = n + 1;
}
```

Figure 1. Pseudo code of parallel recombinative simulated annealing

Initially, we set a sufficiently high initial temperature T for exploring the solution space. The initial population $P(0) = \{X_1(0), X_2(0),\ldots., X_N(0)\}$ of the decision variable values is randomly generated. N is the population size. $X_1(0)$ represents the first optimal solution in the initial population. It is decoded as a binary string. The binary string length is determined by the number and the precision of the decision variables. The cost of each optimal solution is evaluated by cost function. The next generation of optimal solutions is produced by three processes: crossover, mutation and Boltzmann trial. These processes are repeated N/2 times to generate the N optimal solutions of the next generation. For this, two optimal solutions of the initial population are selected as parents. Using the crossover and mutation operators of GAs, two parents produce two children. Then, we evaluate, $C_{children}$, the cost of the children. Two Boltzmann trials are held between parents and children. A Boltzmann trial refers to a competition between the optimal cost of parents and children. A parent has a $1/[1+\exp((C_{parent}-C_{child})/T)]$ probability of wining this trial. A high initial temperature T will be used to ensure that both parent and child are equally likely to win the trial even when a child is a much better optimal solution (lower cost) than a parent, $C_{parent} >> C_{child}$. This acts similarly to the SA Metropolis criterion that allows an uphill move to escape local optimal solutions. The winner of a trial is chosen as a optimal solution for the next generation. After G evolved generations, we reduce the temperature using the SA temperature update function. As T decreases, uphill moves become more difficult. At low temperature, the optimal solution that increases cost has little chance to win the Boltzmann trial. The stopping criterion of PRSA is the final temperature T_f. The algorithm terminates when the temperature T_f is passed.

MANAGEMENT MODEL

Minsker and Shoemaker (1996) proposed dynamic optimal control via successive approximation linear quadratic regulator (SALQR), to optimize in-situ bioremediation design. They developed an optimal control model which combined SALQR and a finite element biodegradation simulation called Bio2D. Optimal results show that time-varying pumping strategy reduced the cost of in-situ bioremediation by 30 % compared with the steady pumping strategy during two-year cleanups (Minsker, 1995). Their cost function considers pumping operation, maintenance, oxygen addition, and treatment costs. It did not include well installation and facilities capital costs. This type of objective function may not be suitable for many in-situ bioremediation system design problems. During a short groundwater remediation, capital costs can dominate total system cost. For example, Culver and Shoemaker (1997) demonstrate that capital treatment costs significantly impact a time-varying pumping strategy of pump-and-treat system for a short management period.

Here, fixed costs of well installation, injection and treatment facilities are included in the objective function. The objective is to minimize the sum of well installation costs, facility capital costs, and operation costs.

$$\text{Minimize} \sum_{\hat{e}=1}^{M^p} [\, C^p(\hat{e})\, p(\hat{e}) + C^{IP}(\hat{e})\, IP(\hat{e}) \,] + D\Big(\sum_{\hat{e}=1}^{M^i} p(\hat{e})\Big) + E\Big(\sum_{\hat{e}=1}^{M^e} p(\hat{e})\Big) \qquad (1)$$

where $\hat{e}$ = index denoting a potential injection or extraction location; $p(\hat{e})$ = injection or extraction rate at location $\hat{e}$ (L^3/T); $C^p(\hat{e})$ = cost coefficient for injection (including oxygen, nutrient and pumping costs) or extraction (including treatment and pumping operation costs) ($ per L^3/T); M^p = total number of injection and extraction wells; $C^{IP}(\hat{e})$ = injection or extraction well installation cost at location $\hat{e}$ ($ per well); $IP(\hat{e})$ = zero-one integer for injection or extraction well existence at location $\hat{e}$; $D\big(\sum_{\hat{e}=1}^{M^i} p(\hat{e})\big)$ = oxygen and nutrient injection facility capital cost, a function of total injection rate ($); M^i = total number of injection wells; $E\big(\sum_{\hat{e}=1}^{M^e} p(\hat{e})\big)$ = treatment facility capital cost, a function of total extraction rate ($); M^e = total number of extraction wells; and $M^p = M^i + M^e$.

Capital cost of injection facility D can be expressed as

$$D\Big(\sum_{\hat{e}=1}^{M^i} p(\hat{e})\Big) = 0 \quad \text{if} \quad \sum_{\hat{e}=1}^{M^i} p(\hat{e}) = 0$$

$$= D_q \quad \text{if} \quad CD_{q-1} < \sum_{\hat{e}=1}^{M^i} p(\hat{e}) \le CD_q \quad q = 1, 2, \ldots\ldots, Q \qquad (2)$$

where D_q = capital cost of injection facility when total injection rate is between design injection capacity CD_{q-1} and CD_q; and Q is the total number of alternative design injection capacities. Injection capacity CD_0 is 0.

Capital cost of treatment facility E can be expressed as

$$E\Big(\sum_{\hat{e}=1}^{M^e} p(\hat{e})\Big) = 0 \quad \text{if} \quad \sum_{\hat{e}=1}^{M^e} p(\hat{e}) = 0$$

$$= E_m \quad \text{if} \quad CE_{m-1} < \sum_{\hat{e}=1}^{M^e} p(\hat{e}) \le CE_m \quad m = 1, 2, \ldots\ldots, M \qquad (3)$$

where E_m = capital cost of treatment facility when total extraction rate is between design treatment capacity CE_{m-1} and CE_m; and M is the total number of alternative design treatment capacities. Treatment capacity CE_0 is 0.

The management model constraints include the following:

1. Upper and lower bounds on injection and extraction rates

$$p^L(\hat{e}) \le p(\hat{e}) \le p^U(\hat{e}) \quad \text{for } \hat{e} = 1,\ldots,M^p \qquad (4)$$

where ^{L} and ^{U} denote lower and upper bound for the variable having the superscript.

2. Bounds on aquifer potentiometric head at injection and extraction wells

$$h^L(\hat{e}) \le h(\hat{e}) \le h^U(\hat{e}) \quad \text{for } \hat{e} = 1,\ldots,M^p \qquad (5)$$

where $h(\hat{e})$ = potentiometric head for injection or extraction well at location $\hat{e}$ [L].

3. Achieving cleanup standard

$$C_{k,T} \le C_{max} \qquad \forall k \in \Psi \qquad (6)$$

where $C_{k,T}$ = contaminant concentration at node k in the end of remediation time T (M/L^3); C_{max} = contaminant concentration of cleanup standard (M/L^3); and Ψ = a set of locations where cleanup standard concentration are enforced. In this study, Ψ includes all nodes of modeling area.

4. Preventing unacceptable concentration migration

$$C_{o,T} \le C_a \qquad \forall o \in \Omega \qquad (7)$$

where $C_{o,T}$ = allowable contaminant concentration at node o in the end of remediation time T (M/L^3); C_a = allowable contaminant concentration (M/L^3); and Ω = a set of monitoring wells.

APPLICATION

Our hypothetical study area is illustrated in Figure 2. It presents the initial contaminant plume and the potential well locations considered by the optimization. Biodegraded contaminant concentrations range to 50 ppm.

The study area is 540 m by 720 m. The homogeneous aquifer has a hydraulic conductivity 6 x 10^{-3} cm/sec and 15 m thickness. To the West and East are fixed head boundaries. To the North and South are no-flow boundaries. Seven wells within the plume can potentially inject water containing 8 mg/l oxygen at rates between 0 and 20 gpm (1.26 liter/sec). Downgradient of the plume six wells can potentially extract contaminated groundwater at rates between 0 and 20 gpm. The cleanup standard, C_{max} , is 3 ppm for the entire study area. Eight monitoring wells are used to observe whether the plume is captured for a three year remediation period (T). The maximum allowable contaminant concentration for monitoring wells, C_a , is 1 ppm.

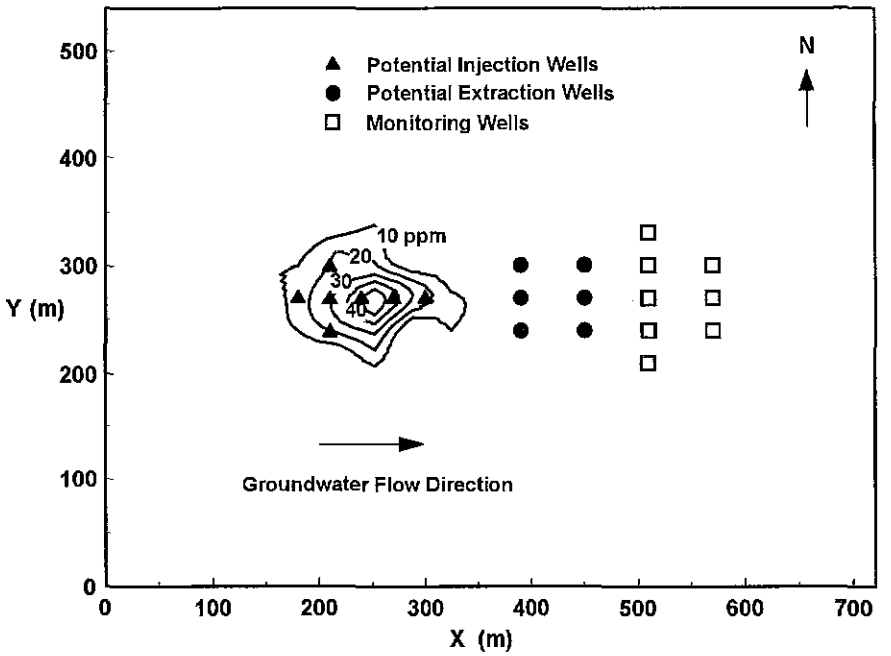

Figure 2. Proposed in-situ bioremediation system and initial contaminant plume

RESULTS

The optimal in-situ bioremediation system design obtained by PRSA is illustrated in Figure 3. Optimization selected five injection and two extraction wells. The optimal total injection and extraction rates are 35.79 gpm (2.26 liter/sec) and 14.75 gpm (0.93 liter/sec), respectively. The optimal strategy reduces contaminant concentration below 3 ppm. The in-situ bioremediation system removed 88% of the initial contaminant mass from the aquifer. Two installed extraction wells prevent the contaminant plume from reaching the monitoring wells. Total system installation and operation cost derived by PRSA is about $251,600.

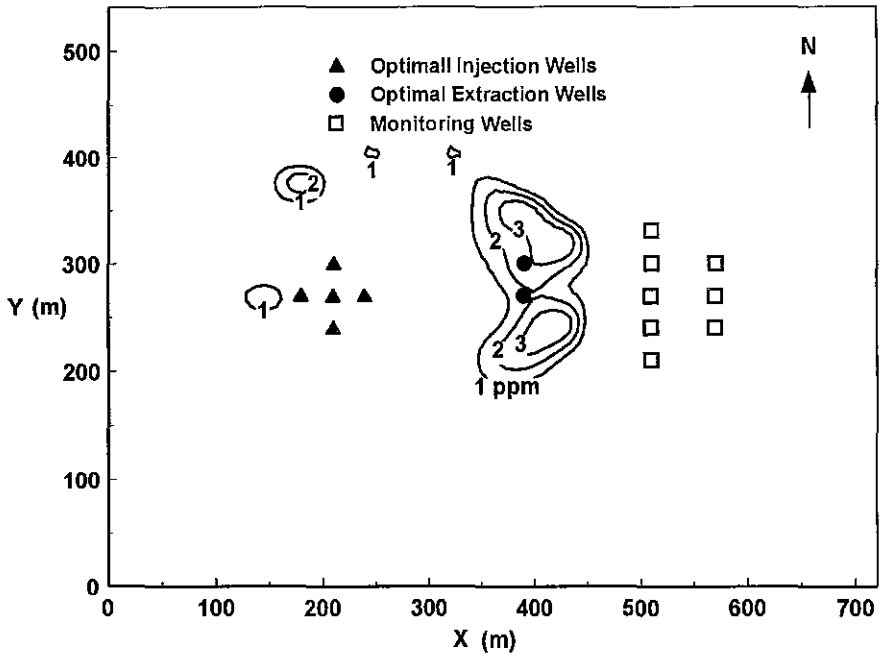

Figure 3. Contaminant plume after 3 years of in-situ bioremediation

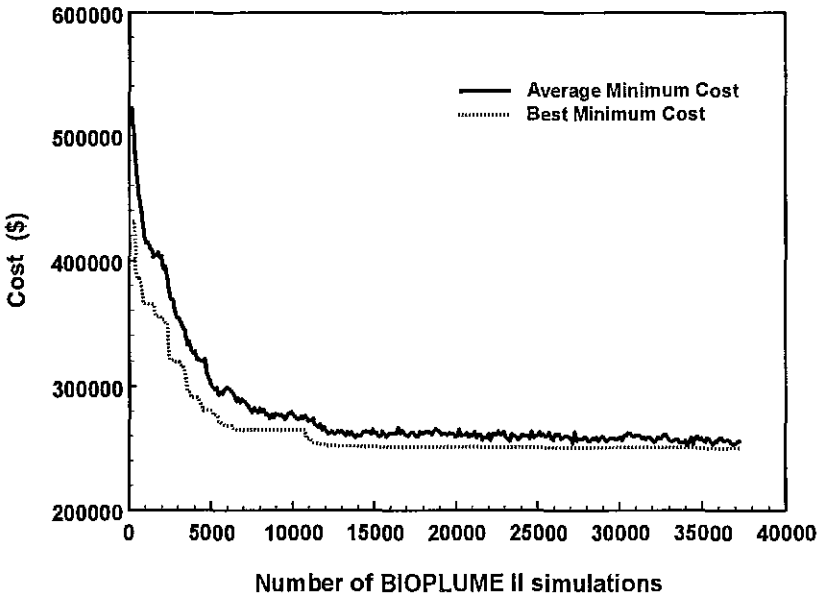

Figure 4. Average minimum cost and best minimum cost vs. number of BIOPLUME II simulations

Figure 4 illustrates the change of the average minimum cost and the best minimum cost at each temperature versus the cumulative number of

BIOPLUME II simulations. Average minimum cost is defined as the average cost of the population for a specific temperature after a certain number of simulations. Best minimum cost is defined as the minimum cost achieved for current or higher temperatures since the algorithm began searching for an optimal pumping strategy. In this study, each pumping rate is decoded as a 10-bit binary code ($2^{10} = 1024$ possible pumping rates). For 13 extraction and injection wells there are 1024^{13}, 1.36×10^{39}, possible pumping strategies. We needed only 37,260 model simulations to obtain the optimal strategy having the best minimum cost of \$251,600 and average minimum cost of \$256,200. After 12,300 simulations, a minimum cost of \$ 252,600 is attained. The additional 24,960 simulations only reduce total cost \$1,000.

The advantage of PRSA is its ability to control the convergence of optimal solutions using an annealing schedule. Figure 5 illustrates the change of the average minimum cost versus temperature using two different annealing parameter values. The temperature function is $T(n+1) = \alpha\ T(n)$. Utilized α values are 0.97 and 0.99. Initial temperature is 50,000. The PRSA algorithm terminated at temperature 1,000. For $\alpha = 0.97$ average minimum cost decreases more slowly than for $\alpha = 0.99$ and 15,660 BIOPLUME II model simulations are needed to reach final average minimum cost of \$267,800. For $\alpha = 0.99$ 37,260 model simulations are needed to reach a final average minimum cost of \$256,200. Accepting a 5% cost increase can save up to 58% of computational cost. This demonstrates the trade-off between computation cost and optimal solution quality.

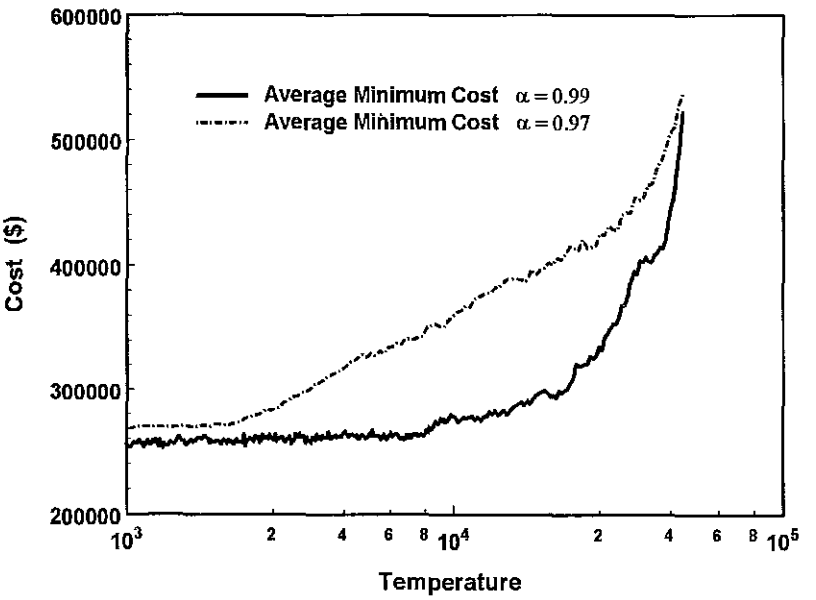

Figure 5. Average minimum cost vs. temperature

Table 1 contrasts two pumping strategies to illustrate the impact of capital costs on the pumping strategy. Strategy A uses equation (1) for its objective function. Strategy B uses equation (8) for its objective function to minimize only total injection and treatment costs.

$$\text{Minimize} \sum_{\hat{e}=1}^{M^P} [\, C^p(\hat{e})\, p(\hat{e}) \,] \qquad (8)$$

After developing pumping Strategy B we estimated the total cost of implementing this strategy. Table 1 shows those values as well as the values computed for Strategy A. Optimal pumping Strategy B requires approximately the same amount ($114,800) for the injection and treatment costs as Strategy A ($112,600). However total system installation and operation costs for Strategy B are 10 % greater than those for Strategy A. The major difference is that Strategy B requires installing six injection wells and four extraction wells. Strategy A only needs five injection wells and two extraction wells.

Table 1. Cost comparison of two pumping strategies

Management formulation	Pumping Strategy A (Optimal pumping strategy considering well installation and capital costs)	Pumping Strategy B (Optimal pumping strategy developed without considering well installation and capital costs)
Injection and treatment costs	$ 112,600	$ 114,800
Well installation cost	$ 84,000	$ 120,000
Treatment facility capital cost	$ 30,000	$ 30,000
Injection facility capital cost	$ 25,000	$ 25,000
Total system cost	$ 251,600	$ 289,800

CONCLUSIONS

We present a simulation/optimization model for optimizing in-situ bioremediation system design. Simulation results predict that the computed optimal design and pumping strategy will reduce contaminant concentration

to the cleanup standard and will prevent contaminant plume migration. For the tested example, in-situ bioremediation system capital cost significantly impacts optimal pumping strategy selection. Considering capital cost in the optimization can reduce well installation costs and considerably reduce total cost.

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