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

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Abstract

Presented is a simulation/optimization (S/O) model combining optimization with BIOPLUME II simulation for optimizing in-situ bioremediation system design. The (S/O) model uses parallel recombinative simulated annealing to search for an optimal design and applies 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. We propose a two-stage management approach. The first stage design goal is to minimize total system cost (pumping/treatment, well installation and facility capital costs). The second stage design goal is to minimize cost of a time-varying pumping strategy using the optimal system chosen by the first stage optimization. Optimization results show that parallel recombinative simulated annealing performs better than simulated annealing and genetic algorithms for optimizing system design when including installation costs. New explicit well installation coding improves algorithm convergence. Threshold accepting reduces

computation time 43 % by rejecting expensive system designs. Applying the optimal time-varying pumping strategy in the second stage reduces pumping cost by 31%.

Key Words: in-situ bioremediation, groundwater remediation, aerobic biodegradation, optimization, parallel recombinative simulated annealing, simulated annealing, genetic algorithm.

INTRODUCTION

In-situ bioremediation for contaminated groundwater cleanup has emerged as a viable remediation technology because of cost-effectiveness and ability to achieve complete destruction of organic contaminants. Many successful applications of in-situ bioremediation for cleaning up petroleum hydrocarbons such as benzene, toluene, ethylbenzene, and xylene (BTEX) have been documented (Flathman, 1993; Hinchee et al., 1994). Major advantages of in-situ bioremediation include (1) lower capital cost, (2) in-situ operation, (3) permanent elimination of contaminants, and (4) cost-effectiveness [Cookson, 1995; Sturman et al., 1995]. An in-situ bioremediation system consists of subsurface delivery systems (injection wells, infiltration galleries or trenches) and recovery wells [Norris et al., 1994]. The recharged water provides sufficient nutrients (e.g. N and P) and electron acceptors (e.g. O_2, NO_3^{-1}, $SO4^{-2}$, Fe^{+3} and CO_2) to stimulate the growth of microorganisms that can transform the contaminants to less harmful chemicals or mineral end products [Alexander, 1994]. Downgradient recovery wells extract contaminated groundwater to contain the plume and to enhance movement of electron acceptors and nutrients. Air stripper tower or activated carbon can treat contaminated groundwater from the recovery wells.

Taylor and Jaffe [1991] applied a bioremediation model to evaluate in-situ bioremediation design for sorbing and nonsorbing contaminants. Lang et al. [1997] designed in-situ bioremediation systems relying on cometabolic degradation. These approaches only employ bioremediation models to evaluate the efficiency of alternative system designs. It is difficult to use a simulation model alone to develop a least cost management strategy when designing a remediation system. A simulation/optimization (S/O) management model, which incorporates a groundwater flow and transport simulation model with an optimization program, can help engineers design an in-situ bioremediation system that satisfies best management goals and regulator requirements.

Many S/O applications have focused on optimal pump-and-treat (P&T) system design [Gorelick et al., 1984; Ahlfeld et al., 1988; Ahlfeld, 1990; Culver and Shoemaker, 1992; Xiang et al., 1995]. Many optimization techniques have been applied within groundwater simulation/optimization management models. Traditional optimization methods include linear programming, nonlinear programming, dynamic programming, quadratic programming, mixed-integer programming. New optimization techniques include simulated annealing [Dougherty and Marryott, 1991; Kuo et al., 1992; Marryott et al., 1993; Marryott, 1996, Rizzo and Dougherty, 1996], neural network [Rogers and Dowla, 1994; Rogers et al., 1995; Johnson and Rogers, 1995] and genetic algorithm [Ritzel et al., 1994; McKinney and Lin, 1994; Huang and Mayer, 1997]. These new techniques eliminate the requirement of computing derivatives with respect to decision variables. Such derivatives are difficult to calculate analytically or numerically in highly nonlinear and noncovex groundwater remediation problems. The new techniques are robust and easily coupled with groundwater simulation models.

McKinney and Lin [1994] applied genetic algorithms (GAs) to develop groundwater management strategies for goals of maximizing pumping, minimizing cost of pumping and minimizing cost of aquifer remediation. Their results show that genetic algorithms can obtain optimal solutions that are as good as or better than those solved by linear and nonlinear programming. GA advantages include straight- forward formulation and no requirement for computing derivatives. GAs using parallel programming can take advantage of network or multi-processors computers to accelerate solution convergence. However, Cieniawski et al. [1995] pointed out some shortcomings. First, the GA requires substantial CPU time for objective function evaluations. Second, it handles multiple constraints with difficulty. Third, GAs are not theoretically guaranteed to find global optimal solutions.

Rogers and Dowla [1994] used artificial neural networks (ANNs) with parallel solute transport modeling to optimize aquifer pump-and-treat remediation. Their approach includes: (1) training an ANN to predict remediation outcome of groundwater flow and transport modelling, (2) using the trained ANN linked with a GA to search through many pumping strategies and select the one which minimizes total pumping while meeting remediation goals. In their groundwater remediation applications, Rogers et al. [1995] treated the pumping rate of each well as either 1 (full capacity pumping) or 0 (no pumping). This reduces the number of groundwater flow and transport simulations needed to train an ANN to predict remediation outcome, but is impractical for real-world applications. Rogers and Dowla [1994] planned to apply ANNs to deal with continuous pumping. However, the computation efficiency and ability of ANNs to find optimal solutions for continuous pumping problems are still unknown.

Dougherty and Marryott [1991] first apply simulated annealing (SA) to groundwater management problems. Marryott [1996] optimizes groundwater remediation design of interceptor trench, slurry wall and low permeability cap using SA. Those SA groundwater management applications assume a discrete solution space. Pumping rates were treated as discrete decision variables. SA has advantages similar to GA. SA is easily implemented with groundwater simulation models and does not require derivative computation. In addition, SA convergence to globally optimal solutions has been proven using homogeneous Markov chain and inhomogeneous Markov chain theory [Geman and Geman, 1984; Hajek, 1988; Romeo, F. and A. Sangiovanni-Vincentelli, 1991]. Because SA sequentially searches for an optimal solution, applying parallel programming to accelerate convergence speed is more difficult with SA than with GA.

We propose applying a new optimization algorithm, parallel recombinative simulated annealing (PRSA), to optimize in-situ bioremediation system design. Mahfound and Goldberg [1995] introduced PRSA as an effective combination of SA and GAs. PRSA retains the desirable asymptotic convergence of SA and adds the GA's population approach and recombinative operator. Here, we present the first application of PRSA to in-situ bioremediation or groundwater management system design. The manuscript is organized as follows. In section 2, we formulate the management problem and describe the two-stage management approach. In section 3, we provide an overview of PRSA and its implementation. We also propose new techniques to improve PRSA performance. These techniques include Gray coding, uniform crossover, threshold accepting function and segregated genetic algorithm. In sections 4 and 5, we briefly introduce the bioremediation simulation model and describe the system design study case. In sections 6 and 7, we demonstrate in-situ bioremediation system design by PRSA and summarize findings.

OPTIMAL SYSTEM DESIGN OF IN-SITU BIOREMEDIATION

Minsker and Shoemaker [1996] proposed dynamic optimal control via successive approximation linear quadratic regulator (SALQR), to optimize in-situ bioremediation design. Their optimal time-varying pumping strategy reduced the cost of in-situ bioremediation by 30 % compared with a steady pumping strategy during two-year cleanups [Minsker, 1995]. Their cost function considered pumping operation, maintenance, oxygen addition, and treatment costs. It did not include well installation and facilities capital costs – costs which can dominate in-situ bioremediation or P&T system costs for a short remediation period. Culver and Shoemaker [1997] demonstrate that capital treatment costs significantly affect a time-varying 5-year P&T pumping strategy period. They recommend explicitly incorporating these capital costs into a dynamic management model.

In this study, we propose a two-stage design approach. The first stage optimizes in-situ bioremediation system configuration, including the pumping well locations, steady pumping rates and facility capacities; the objective is to minimize total system cost including pumping/treatment, well installation, and facilities capital costs. The second stage involves reducing pumping costs of the system designed in the first stage; the objective is minimize pumping cost plus facility capital cost using a time-varying pumping strategy.

The first stage objective function is expressed as

$$\text{Minimize} \quad Z = W_1 \sum_{\hat{e}=1}^{M^p} C^p(\hat{e})\, p(\hat{e}) + W_2 \sum_{\hat{e}=1}^{M^p} C^{IP}(\hat{e})\, IP(\hat{e})$$

$$+ W_3\, D\Big(\sum_{\hat{e}=1}^{M^i} p(\hat{e})\Big) + W_4\, E\Big(\sum_{\hat{e}=1}^{M^e} p(\hat{e})\Big) \qquad (1)$$

where Z = total present worth of in-situ bioremediation system; W_1, W_2, W_3, and W_4 are factors used to convert pumping/treatment costs, well installation costs, injection facility capital cost and treatment facility cost to their present value, respectively; $W_1 = [(1+i)^{Te}-1]/[i(1+i)^{Te}]$; i is a discount rate and Te is total duration of remediation period; W_2, W_3, and W_4 are equal to 1; $\hat{e}$ = 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 $\hat{e}$; $D(\sum_{\hat{e}=1}^{M^i} p(\hat{e}))$ = oxygen and nutrient injection facility capital cost, a function of total injection rate ($); M^i = total number of injection wells; $E(\sum_{\hat{e}=1}^{M^e} p(\hat{e}))$ = treatment facility capital cost, a function of total extraction rate ($); M^e = total number of extraction wells; and $M^p = M^i + M^e$.

Injection and treatment facilities capital cost is dependent on facility capacities. In practical engineering design, facility capital cost is not a continuous function of capacity because only specific sizes on models of pipes, pumps and facilities are manufactured. Therefore, we use discrete function to present these facility capital costs. Capital cost of injection facility D can be expressed as

$$
\begin{aligned}
D\Big(\sum_{\hat{e}=1}^{M^i} p(\hat{e})\Big) &= 0 \quad \text{if} \quad \sum_{\hat{e}=1}^{M^i} p(\hat{e}) = 0 \\
&= D_q \quad \text{if} \quad CD_{q-1} < \sum_{\hat{e}=1}^{M^i} p(\hat{e}) \le CD_q \quad q = 1, 2, \ldots.., M^Q \qquad (2)
\end{aligned}
$$

where D_q = capital cost of injection facility when 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. The equation defining treatment facility E capital cost is analogous to Eq (2) and obtained by substituting $E(\sum_{\hat{e}=1}^{M^e} p(\hat{e}))$ for

$D(\sum_{\hat{e}=1}^{M^i} p(\hat{e}))$, M^e 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 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.

The first management objective function is a combination of mixed-integer programming (well installation cost) and combinatorial optimization (discrete facility capacity). Traditional optimization techniques such as mixed-integer nonlinear programming cannot apply to equation (1) which is not differentiable. An advantage of SA, GA and PRSA is they do not need function derivatives

First and second stage management model constraints include the following:

1. Upper and lower bounds on injection and extraction rates
2. Bounds on aquifer hydraulic heads at injection and extraction wells
3. Upper bound on final contaminant concentration needed to achieve a cleanup standard

$$C_{k,\,Te} \leq C_{cl} \qquad \forall k \in \Psi \tag{3}$$

where $C_{k,Te}$ = contaminant concentration at node k by the end of time period Te (M/L^3); C_{cl} = 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 study area nodes.

4. Upper bound on concentration at specific locations to assure capture (prevent unacceptable concentration migration)

$$C_{o,t} \le C_{ca} \qquad\qquad \forall o \in \Omega \qquad\qquad (4)$$

where $C_{o,t}$ = contaminant concentration resulting at node o by the end of period t (M/L^3); C_{ca} = maximum allowable contaminant concentration (M/L^3); and Ω = a set of monitoring wells.

In the second stage, we plan to use the wells suggested for installation by the first stage. However, in this stage we minimize the cost of injection, extraction and treating water at time-varying rates. We must consider the injection and treatment facility costs since those are functions of pumping rates. Thus, the second stage objective function is:

$$\text{Minimize} \quad U = \sum_{t=1}^{M^n}\left(\frac{1}{(1+i)^{t y_p}} \sum_{\hat{e}=1}^{M^p} C^p(\hat{e})\, p(\hat{e},t)\right)$$

$$+ W_3 \,\text{Max}\left\{D\left(\sum_{\hat{e}=1}^{M^i} p(\hat{e},t)\right)\right\}_{t=1}^{M^n} + W_4 \,\text{Max}\left\{E\left(\sum_{\hat{e}=1}^{M^e} p(\hat{e},t)\right)\right\}_{t=1}^{M^n} \qquad (5)$$

where U = total present worth of pumping and facility capital costs; $p(\hat{e},t)$ = injection or extraction rate at location ê for stress period t (L^3/T) (a stress period is a period of unchanging pumping); M^n = total number of stress periods; y_p = stress period duration (T). Injection and treatment facilities are constructed before enhanced bioremediation commences. Facility capital costs are determined by the capacity requirement. Injection and treatment facility capacities must not be less than the greatest total injection and extraction rates, respectively. The second phase S/O model employs the same constraints as the first phase.

PARALLEL RECOMBINATIVE SIMULATED ANNEALING

Simulated Annealing and Genetic Algorithms

The study of GAs has been well documented by many researchers [Holland, 1975; Goldberg, 1989; Davis, 1991; Michalewicz, 1992; Mitchell, 1996; Bäck, 1996; Bäck et al.,1997]. GAs 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 multireservoir operation [Oliveira and Loucks, 1997]. 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 lack good control of convergence.

On the other head, SA can be mathematically proven to converge to global optimal solutions. The proof mainly depends on the annealing schedule. By slowly decreasing the 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 paralleling simulated annealing to accelerate convergence very difficult. Recently, researchers have investigated hybrid genetic annealing algorithm (GAA) approaches that combine desirable attributes of GA and SA methods [Sirag and Weisser, 1987; Brown et al., 1989; Boseniuk and Ebeling, 1991; Lin et al., 1993; Chen and Flann, 1994; Mahfound and Goldberg, 1995; Yong et al., 1995; Varanelli and Cohoon, 1995; Jeong and Lee, 1996]. The intended result is a general-purpose optimization algorithm that has the good SA convergence control and the efficient GA parallelization. Chen and Flan [1994] investigated 14 hybrid methods of combining GA and SA. For nine optimization problems, combining GA crossover and mutation operators with SA annealing schedule has yielded the best performance. Varanelli and Cohoon [1995] used population-oriented simulated annealing (POSA) to solve a VLSI network partitioning problem. Their results showed that POSA converged to a better optimal solution than GA for the same CPU time.

Goldberg [1990] introduced the annealing schedule and the Boltzmann distribution to help prove GA convergence to global optimality. Mahfound and Goldberg [1995] presented a parallel recombinative simulated annealing (PRSA) algorithm and proved its asymptotic global convergence. For their test problems, PRSA consistently converged to the global optimum. The PRSA algorithm effectively combines simulated annealing and genetic algorithms to offer the user control over convergence.

Implementation of PRSA

PRSA implementation is illustrated in Figure 1. Initially, we set a sufficiently high annealing temperature T_0 for exploring the solution space. Annealing temperature is a control parameter of PRSA convergence.

The initial population P^0 of the decision variable values = (X_1^0, X_2^0, X_3^0, ……, X_N^0), is randomly generated. N is the population size. X_1^0 represents the first system configuration in the initial population. It is coded as a binary string. The precision of a decision variable value determines its binary string length. System configuration costs are represented by cost function.

A new generation of system configurations is produced by three processes: crossover, mutation and Boltzmann trial. These processes are repeated N/2 times to generate the N new system configurations of the next generation P^{k+1}. In more details, two system configurations from the previous population (P^k) are chosen as parents without replacement. Using the crossover and mutation operators of GA, two parents produce two children. Then, the system costs of the two children are evaluated. Two Boltzmann trials are conducted. A Boltzmann trial refers to a competition between the system costs of a parent and a child. A parent has a $1/[1+\exp((C_{parent}-C_{child})/T_n)]$ probability of wining this trial. A high initial temperature T_0 is used to ensure that both parent and child are equally likely to win the trial even if a child is a much better solution (lower cost) than a parent, $C_{parent} << C_{child}$. This allows what is termed an uphill move in the decision space to permit escape from local optimal solutions. The winner of a trial is selected (as an optimal solution) for use as a parent of the next generation. After G

evolved generations, we reduce the temperature using the SA temperature update function $T_{n+1} = \alpha T_n$. As T_{n+1} decreases, uphill moves become more difficult. At low temperature, a system configuration that increases cost has little chance to win the Boltzmann trial because of low probability. The stopping criterion of PRSA is a final temperature T_f. The algorithm terminates when temperature T_f is passed.

Improvement of PRSA

New SA or GA techniques can potentially improve PRSA performance. Sample techniques are (1) Gray coding scheme, (2) explicit well installation coding, (3) uniform crossover, (4) threshold accepting function, and (5) segregated genetic algorithm.

Most GA encoding scheme use binary strings (0 and 1 bits) to represent decision variables [Holland, 1975]. Some researchers suggested real-valued coding (floating point representation) for real parameter optimization to increase efficiency and numerical precision [Wright, 1991; Goldberg, 1991; Janikow and Michalewicz, 1991; Eshelman and Schaffer, 1993; Surry and Radcliffe, 1997]. In this study, we choose Gray coding as the coding scheme of PRSA.

Gray coding can help in the following manner. Although Gray coding uses 0 and 1 bits to represent decision variables, it is an improvement because it reduces Hamming distance to 1 for adjacent decision variables. Hamming distance is defined as the number of bits difference between neighborhood substrings. The Gray code ensures that two similar solutions are represented by two similarly coded strings. Hinterding et al. [1995] found Gray code performance usually superior to binary code for function optimization.

Dandy et al. [1996] use Gray code to improve GA performance for pipe network optimization. Rana and Whitley [1997] prefer Gray coding for bit representation in GA.

In groundwater remediation design involving well installation, installation cost is usually treated as an implicit decision variable such that well installation cost is zero if pumping rate is zero or close to zero [McKinney and Lin, 1995; Sawyer and Ahlfeld, 1995]. Huang and Mayer [1997] use well locations as explicit decision variables in P&T GA optimization. They encode the x and y coordinates of well locations into a GA substring. Their objective is to minimize P&T cost by optimizing well locations and pumping rates simultaneously, but well installation cost is still determined by pumping rate (i.e. no well installation if pumping rate is zero).

Here we propose a new approach which we termed explicit well installation coding. Each pumping well installation is explicitly coded as 1 or 0 bit values representing whether the well is or is not installed, respectively. Initially, PRSA randomly generates system configurations indicating injection and extraction well installation. Using crossover, mutation, and Boltzmann trial, PRSA optimizes the number of installed pumping wells and pumping rates to minimize system cost.

Crossover, mutation and selection are three important GA operators. Two parent solutions use crossover and mutation to create two child solutions. Then, the selection operator selects solutions from the current population to form the next evolved generation. Mutation is usually a background operator in GA. The two main operators are crossover and selection. Traditional crossover operators are one-point and two-point crossover [Goldberg, 1989]. We choose uniform crossover for PRSA because Syswerda

[1989] shows that uniform crossover is superior to one-point and two-point crossover theoretically and empirically. In GA water resources applications, uniform crossover applications include water distribution networks design [Savic and Walters, 1997] and multireservoir operation [Oliveira and Loucks, 1997].

Traditional GA selection operators include proportional, tournament, ranked-based selections [Bäck et al.,1997]. However, PRSA employs Boltzmann trial as its selection operator [Mahfound and Goldberg, 1995]. A Boltzmann trial uses annealing temperature to control selection pressure, which is described previously. To reduce S/O model simulation requirements, we introduce a threshold accepting function (TAF) [Dueck and Scheuer, 1990; Moscato and Fontanari, 1990; Althofer and Koschnick, 1991] to reject expensive system design without requiring additional simulations. We will contrast the optimization results of Boltzmann trial and TAF for in-situ bioremediation system design application.

This TAF (Figure 2) uses a deterministic rule to accept or reject a new configuration. Total cost now includes total system and penalty costs. The penalty cost is based on constraints violated according to biodegradation model simulation. After the crossover and mutation operators generate a new configuration (child), we calculate $C_{child\ system}$ (child system cost) and ΔC_{system}, ($C_{parent\ system}$-$C_{child\ system}$), or the difference between parent and child system costs. If (ΔC_{system}-parent penalty cost) is larger than the current temperature T_n, the new configuration is automatically rejected. Under this condition, it is not necessary to run the simulation model because the new configuration has no chance to be accepted at the current T_n even if the new penalty cost is zero. If (ΔC_{system}-parent penalty cost) is smaller than current T_n (i.e. new configuration reduces the system cost, or new configuration increases the system cost but has a chance to be accepted), we run the simulation model and estimate a child penalty cost. ΔC, (C_{parent}-C_{child}), is calculated. TAF is used again to determine whether to accept or reject the new configuration.

Constraint handling is an important issue for many design problems. Michalewicz and Schoeauer [1996] review constraint handling methods applied in evolutionary algorithms. Most of these methods employ penalty functions that penalize infeasible solutions. Here we deal with inequality constraints by expanding the objective function to include penalty cost for infeasible solutions. A penalty cost function is defined as

$$\begin{aligned} f_j(X) &= Pe(j)\, g_j(X) \quad && \text{for violated constraint } g_j(X) > 0 \\ &= 0 && \text{for satisfied constraint } g_j(X) \le 0 \end{aligned} \tag{6}$$

where $f_j(X)$ is a penalty cost function for j^{th} constraint ($g_j(X) \le 0$); $Pe(j)$ is a penalty coefficient for j^{th} constraint. The penalty cost is calculated by the distance from feasibility (acceptability) multiplied by a penalty cost coefficient for the violated constraint (i.e. if $g_j(X) > 0$). If the constraint is satisfied (i.e. if $g_j(X) \le 0$), the penalty cost is zero.

Specifying penalty coefficients is challenging. A high penalty coefficient will ensure most solutions lie within the feasible solution space, but can lead to costly conservative system designs. A low penalty coefficient permits searching both feasible and infeasible regions, but can cause convergence to an infeasible system design.

Le Riche et al. [1995] introduce a segregated genetic algorithm to reduce penalty weight influence. The segregated GA uses two penalty coefficient values instead of one. It maintains two populations: individuals selected from a large penalty population will more likely stay in the feasible region; individuals selected from a small penalty population will probably remain in the infeasible region. Eventually, the optimization algorithm will converge to the feasible optimum from both sides of the feasible region boundary. We adapted this segregated method to PRSA procedures:

Step 1. Generate two parent populations randomly. Evaluate the objective function values of one population using large penalty coefficients. Evaluate the other population using small penalty coefficients.

Step 2. Each parent population uses crossover and mutation to generate its child population.

Step 3. Evaluate the objective function values of child population of large penalty parent population using large penalty coefficients. Evaluate the objective function values of child population of small penalty parent population using small penalty coefficients.

Step 4. New large penalty parent population is selected by competition between the current large penalty parent and child populations using Boltzmann trial or TAF. New small penalty parent population is selected by the competition between the current small penalty parent and child populations using Boltzmann trial or TAF.

Step 5. Exchange individual solutions between the new large penalty and small penalty parent populations.

Step 6. Continue step 2 through step 5 until stopping criterion is satisfied.

GROUNDWATER BIODEGRADATION MODELS

Computer models incorporating microbial growth and biodegradable pollutants transport can be classified according to conceptual approach [Baveye and Valocchi, 1989]. The first approach, which has been applied to biological wastewater treatment, uses a biofilm concept to simulate trace-organics biodegradation in the subsurface [Rittmann et al., 1980]. The second approach assumes contaminant transport and biodegradation occur in small discrete colonies attached to the surface of the solid aquifer particles [Molz et al., 1986]. They assume that a microcolony has the form of a cylindrical plate with radius and thickness and can be viewed as a simplified biofilm model. The third approach is strictly macroscopic and makes no assumption about microorganism distribution within the pore space. Removal of organic contaminant is assumed to be by Monod or Michaelis-Menten kinetics involving aerobic degradation and anaerobic degradation in the subsurface [Borden and Bedient, 1986]. A simplified simulation model using the third approach, BIOPLUME II, assumes that aerobic biodegradation can be treated as an instantaneous reaction [Rifai et al., 1988; Rifai and Bedient, 1990].

The BIOPLUME II model uses a dual-particle mover procedure to simulate subsurface oxygen and contaminants transport. It was developed by modifying a two-dimensional transport model -- the method of characteristics (MOC) model [Konikow and Bredehoeft, 1978] . The contaminant and oxygen transport equations are solved at every time step to calculate contaminant and oxygen distributions [Rifai et al., 1988] :

$$\frac{\partial(Cb)}{\partial t} = \frac{1}{R_c}\left[\frac{\partial}{\partial x_i}(bD_{i,j}\frac{\partial C}{\partial x_j}) - \frac{\partial}{\partial x_i}(bCV_i)\right] - \frac{C'W}{n_e} \tag{7}$$

$$\frac{\partial(Ob)}{\partial t} = \left[\frac{\partial}{\partial x_i}(bD_{i,j}\frac{\partial O}{\partial x_j}) - \frac{\partial}{\partial x_i}(bOV_i)\right] - \frac{O'W}{n_e} \tag{8}$$

where C and O = contaminant and oxygen concentration (M/L^3), respectively; C′ and O′ = contaminant and oxygen concentration in a source or sink fluid (M/L^3); n_e = effective porosity; b = aquifer saturated thickness (L); t = time (T); x_i and y_i = cartesian coordinates (L); W = volume flux per unit area (L/T); V_i = seepage velocity in the direction of x_i (L/T); R_c = retardation factor for contaminant; and $D_{i,j}$ = hydrodynamic dispersion coefficient (L^2/T).

The contaminant and oxygen plumes are combined using superposition to simulate instantaneous reaction between oxygen and the contaminants. Contaminant and oxygen concentration decreases at a node are calculated from

$$\Delta C_{RC} = O/F\ ; \quad O = 0 \text{ if } C > O/F \tag{9}$$

$$\Delta C_{RO} = CF \, ; \quad C = 0 \quad \text{if} \quad O > CF \tag{10}$$

where ΔC_{RC} and ΔC_{RO} = calculated change in contaminant and oxygen concentrations, respectively; F = ratio of consumed oxygen to consumed contaminant.

BIOPLUME II can be calibrated and applied using data such as hydrogeological parameters, contaminant chemical and physical properties, contaminant source concentrations, and background oxygen concentration. Limitations of the BIOPLUME II model are : (1) it is unsuitable for simulating slowly biodegraded contaminants under aerobic condition because of its instantaneous reaction assumption, and (2) it is incapable of simulating anaerobic processes affected by other electron acceptors such as nitrate, ferric iron, sulfate and inorganic carbon. Here we use BIOPLUME II to simulate aerobic biodegradation processes and contaminant transport within a simulation/optimization management model.

STUDY CASE

Figure 3 illustrates the hypothetical study area and the initial contaminant plume. Table 1 presents BIOPLUME II input parameters for the 510 m by 690 m study area. The homogeneous aquifer has a hydraulic conductivity 6 x 10^{-5} m/sec and 15 m aquifer thickness. To the West and East are fixed head boundaries -- 30.5 and 27.7 m, respectively. Groundwater flow is from West to East. The initial hydraulic gradient is 0.004. To the North and South are no-flow boundaries. Groundwater flow simulation is steady state. The contaminant retardation factor is assumed to be 1.

Figure 3 illustrates the plume configuration after 5 years if no action is taken. It will move and expand, reaching the monitoring wells. Natural aerobic decay reduces the total contaminant mass by only 16 %. An in-situ bioremediation system should be installed to contain the contaminant plume and enhance contaminant biodegradation.

To design an in-situ bioremediation system, the optimization will consider potential injection and extraction wells. Seven wells within the plume can potentially inject water containing oxygen and nutrients at rates between 0 and 20 gpm (1.26 liter/sec). Upper and lower bounds of hydraulic head for the injection wells are 33.5 and 27.7 m, respectively. The initial oxygen concentration is 5 ppm except in the contaminant plume area, where the oxygen concentrations have been consumed by aerobic biodegradation. The vertical exchange of oxygen with the unsaturated zone is assumed to be insignificant. The injected oxygen concentration is 8 ppm. BIOPLUME II model assumes that injected water provides enough nutrients to support microbial growth in the aquifer.

Figure 4 illustrates the potential well locations considered by the optimization. Six downgradient wells can potentially extract contaminated groundwater at rates between 0 and 20 gpm. The upper and lower bounds of hydraulic head for the extraction wells are 30.5 and 24.4 m, respectively. The cleanup standard, C_{cl} , is 3 ppm for the entire study area.

Figure 4 also identifies monitoring wells (not subject to optimization) used to observe whether the plume is captured during a three-year remediation period. Because the system can inject potentially much water, additional monitoring wells are installed in

the Western boundary. This helps ensure that unacceptable plume spreading does not result. The maximum contaminant concentration allowed to reach monitoring wells, C_{ca} , is 1 ppm.

Table 2 lists cost coefficients used to estimate system costs. The injection coefficient is based on the nutrients, oxygen and pumping operation costs. The extraction cost coefficient considers cost of treating and pumping contaminated groundwater. Treatment includes air stripping and granular activated carbon. Injection and treatment facilities capital costs are based on their capacities.

APPLICATIONS AND RESULTS

Optimal In-situ Bioremediation System Design with Fixed Cost

The first stage management goal is to minimize total system cost which includes pumping/treatment, well installation, and facilities capital costs. Below we contrast abilities of SA ,GA and PRSA varieties to achieve this goal. In SA we use a threshold accepting function and Corana's neighborhood search [Corana et al., 1987] to reduce SA computation cost and extend its ability to deal with continuous variables. Our two GA formulations are based on the methodology of McKinney and Lin [1994], but include replacing binary code with Gray code and use of uniform crossover. Our GAs also extend tournament size of tournament selection from 2 to 4 to increase selection intensity [Blickle and Thiele, 1996] and to improve convergence. We implement segregated GA to refine search in both feasible and infeasible regions. The parameter choice of GAs and PRSA is problem-dependent. After some test runs, we choose population size 100 for optimizing system design with fixed cost and 200 for minimizing cost of time-varying pumping strategy. Crossover and mutation rates used for GAs and PRSA are 0.9 - 1.0 and 0.01 - 0.03, respectively.

We use six formulations to compare the three optimization algorithms. Because of the stochastic nature of these algorithms, we run each formulation twenty times using different random seeds. Table 3 lists maximum, minimum and average system costs of these runs for six formulations. Figure 5 illustrates the error bars of six formulations. The upper and lower caps indicate the average system cost plus or minus one standard deviation, respectively. The large standard deviation reflects that the optimization algorithm does not converge to the same optimal solution consistently.

PRSA2 (PRSA with Boltzmann trial and explicit well installation) designs the least-cost system (\$188,6 00). It also has the lowest average system cost (\$193,900) and the smallest standard deviation (Figure 5). GA2 and PRSA2 perform well because of explicit well installation coding. GA1 and PRSA1 using implicit well installation do not converge to optimal solutions. It is difficult for GA1 and PRSA1 to reduce well numbers because implicit well installation depends on whether or not pumping rates reach zero. SA1 shows that SA can converge to optimal solutions but is not as stable as PRSA (note the large standard deviation in Figure 5). Threshold accepting helps SA1 and PRSA3 converge to optimal solution using fewer simulations. For example, PRSA3 reduces average number of simulation by 43% compared with PRSA2, while still maintaining reasonably good solution quality (low average system cost and small standard deviation).

Figure 6 shows the convergence behavior of SA, GA and PRSA. It illustrates the change of system cost vs. number of BIOPLUME II simulations as the optimization algorithms progress. We compare the best results of six formulations (minimum system cost of six formulations) in Figure 6. PRSA1 and GA1 converge slowly because of implicit well installation. GA2 has the fastest convergence but additional simulations do not improve solution quality. PRSA2 uses uphill moves (Boltzmann trial) and explicit well installation to gradually converge to optimality. SA1 and PRSA3 employ threshold accepting to reject some expensive system designs without requiring simulation. This reduces total simulations and computation effort. Table 4 compares optimal systems designed by the different approaches. All three algorithms design similar systems. All use three or four injection wells and one extraction well. However, the PRSA yields the least cost strategy.

Time-varying Pumping Strategy

The second stage management goal is to minimize injection, extraction and treatment costs plus facility capital costs that are functions of the flow rates. Employing the four wells (U1, U2, U4 and E1) selected in the first stage optimization, we develop time-varying pumping strategy for a three-year remediation consisting of six half-year pumping periods. Figure 7 contrasts steady and time-varying pumping strategies. Optimal time-varying pumping reduces total injection and extraction volumes by 27 % and total injection and extraction cost by 31% when comparing with the optimal steady-pumping (Table 5). This supports the finding of Minsker [1995] that time-varying pumping can manage in-situ bioremediation better than steady pumping.

Figure 8 shows contaminant plume response to optimal time-varying pumping. The pumping strategy prevents contaminant from reaching monitoring wells and achieves the final 3 ppm concentration cleanup standard. During management periods 1 to 4, injection wells U2 and U4 employ nearly their full pumping capacity 20 gpm (1.26 liter/sec) to enhance contaminant biodegradation [see Figure 7 (b)]. For periods 5 and 6, three injection wells employ low rates below 2 gpm (0.126 liter/sec) because injected oxygen can no longer reach contamination that is moving eastward [see Figure 8 (e) and (f)]. Extraction well E1 begins at a low pumping rate. Later, extraction increases to enhance mixing of oxygen and nutrients with contaminant. During the final periods, the extraction well serves mainly to contain plume migration.

For a short term remediation project, the first stage goal of reducing capital costs is more important than the second stage goal of reducing pumping costs. Table 6 compares pumping volumes and system costs for two cases, A and B. Design A configuration results from the first stage PRSA optimization. Design B is selected based on experience instead of optimization. Design B employs more wells than design A. Design B reduces injection volume by 25% and has lower pumping cost. The four injection and three extraction wells of design B efficiently use injected oxygen for biodegradation. However, $4,400 pumping cost reduction cannot offset the $44,000 fixed cost increase due to additional wells and treatment facility capital costs (Table 6).

This illustrates that minimizing in-situ bioremediation system design while including fixed cost is sometimes more important than merely minimizing time-varying pumping cost.

CONCLUSIONS

We present a parallel recombinative simulated annealing (PRSA) model to optimize in-situ bioremediation system design. The new simulation/optimization model determines the pumping (extraction/injection) strategy that minimizes total system cost, reduces contaminant concentration to cleanup standard, and prevents contaminant plume migration. To improve PRSA convergence and performance we employ Gray code, uniform crossover, explicit well installation coding, threshold accepting function (TAF) and segregated genetic algorithm. Compared with Boltzmann trial, TAF reduces computation cost 43 % by rejecting expensive system design without requiring simulations.

PRSA minimizes total system cost (pumping/treatment, well installation and facility capital costs) better than SA and GA. An optimal time-varying pumping strategy requires 31 % less pumping costs than an optimal steady pumping strategy. Optimizing system design while including fixed costs more significantly impacts total system cost than merely minimizing pumping/treatment costs for the 3-year in-situ bioremediation project.

Parallel recombinative simulated annealing is a general-purpose optimization approach that has the good convergence of SA and the efficient parallelization of GAs.

Here we have shown its efficiency and flexibility for optimizing system installation design and time-varying pumping.

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Table 1. Input parameters of BIOPLUME II simulation model

Input parameter	Value
Grid size	19 × 25
Cell size	30 m × 30 m
Hydraulic conductivity	6×10^{-5} m/sec
Aquifer thickness	15 m
Hydraulic gradient	0.004
Longitudinal dispersivity	10 m
Transverse dispersivity	2 m
Effective porosity	0.3
Retardation factor	1.0
Anisotropy factor	1.0
Injected oxygen concentration	8 ppm
Background oxygen concentration	5 ppm
Remediation time	3 years

Table 2. Cost function coefficients

Coefficients	Value
Discount rate	0.05
C^P for injection cost (oxygen, nutrient and pumping operation)	300 ($ per gpm-year)
C^P for extraction cost (treatment and pumping operation)	1,000 ($ per gpm-year)
C^{IP} (well installation cost)	12,000 ($ per well)
D (injection facility capital cost)	D_{20gpm} = \$ 20,000 D_{40gpm} = \$ 24,000 D_{60gpm} = \$ 28,000 D_{80gpm} = \$ 32,000 D_{100gpm} = \$ 36,000 D_{120gpm} = \$ 40,000 D_{140gpm} = \$ 44,000
E (treatment facility capital cost)	E_{20gpm} = \$ 30,000 E_{40gpm} = \$ 38,000 E_{60gpm} = \$ 46,000 E_{80gpm} = \$ 54,000 E_{100gpm} = \$ 62,000 E_{120gpm} = \$ 70,000

Note : 1 gpm = 0.06309 liter/sec.

Table 3. Optimal system costs for SA, GA and PRSA (20 runs for each formulation)

Formulation	Max ($)	Average ($)	Min ($)	Average number of simulations
SA1	248,386	215,000	197,300	7,767
GA1	315,493	273,900	230,600	13,100
GA2	227,649	209,000	196,500	13,100
PRSA1	280,207	256,600	239,400	13,300
PRSA2	199,333	193,900	188,600	13,300
PRSA3	202,734	196,700	191,900	7,591

SA1 : simulated annealing with continuous variables and threshold accepting
GA1 : genetic algorithm with implicit well installation
GA2 : genetic algorithms with explicit well installation
PRSA1 : PRSA with Boltzmann trial and implicit well installation
PRSA2 : PRSA with Boltzmann trial and explicit well installation
PRSA3 : PRSA with threshold accepting and explicit well installation

Table 4. Optimal system from SA, GA and PRSA

	Well installation cost ($)	Injection cost ($)	Extraction cost ($)	Injection facility capital cost ($)	Treatment facility capital cost ($)	System cost ($)
SA	60,000	36,200	43,100	28,000	30,000	197,300
GA	48,000	38,100	52,400	28,000	30,000	196,500
PRSA	48,000	37,600	44,900	28,000	30,000	188,500

SA employs 4 injection wells (U1,U2,U3, and U4) and 1 extraction well (E2)
GA employs 3 injection wells (U1,U2, and U4) and 1 extraction well (E2)
PRSA employs 3 injection wells (U1,U2, and U4) and 1 extraction well (E2)

Table 5. Pumping volumes and costs comparison of steady and time-varying strategies

	Injection volume (gallon)	Extraction volume (gallon)	Injection cost ($)	Extraction cost ($)
Steady pumping	72,647,793	26,043,548	37,600	44,900
Time-varying pumping	52,376,469	19,195,059	25,800	31,500

Note: 1 gallon = 3.78534 liters

Table 6. Comparison of pumping volumes and system costs for different system designs using time-varying pumping

Design	Injection volume (gallon)	Extraction volume (gallon)	Pumping cost ($)	Well installation and facilities capital cost ($)	System cost ($)
A	52,367,469	19,195,059	57,300	106,000	163,300
B	39,237,938	23,762,873	53,000	150,000	203,000

Design A has 3 injection wells (U1,U2, and U4) and 1 extraction well (E2) which is selected by PRSA optimization.
Design B has 4 injection wells (U1,U2, U3 and U4) and 3 extraction wells (E1,E2,and E3) which is selected based on experience.

```
initialize T0;
initialize P^0 = { X1^0, X2^0, ........ XN^0 } ;
evaluate C^0 = cost function(P^0);
k , n = 0;
while (Tn > Tf)
{
   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);
         if  ( random(0,1) < 1/[1+exp((Cparent-Cchild)/Tn] )
            select Xparent;
         else
            select Xchild;
      }
      P^k+1 = {X1^k+1, X2^k+1, ......, XN^k+1};
      k = k +1;
   }
   Tn+1 = αTn;
   n = n + 1;
}
```

Figure 1. Pseudo code of parallel recombinative simulated annealing

```
C_parent system = Parent System Cost;
C_parent = C_parent system + Parent Penalty Cost;
C_child system = Child System Cost
ΔC_system = C_child system - C_parent system

if (ΔC_system - Parent Penalty Cost <= T_n)
   run simulation model;
   calculate Child Penalty Cost;
   C_child = C_child system + Child Penalty Cost;
   ΔC = C_child - C_parent
   if (ΔC <= T_n)
      return (1); /* accept new configuration */
   else
      return (0); /* reject new configuration */
else
   return (0); /* reject new configuration */
```

Figure 2. Pseudo code of threshold accepting function applied to optimal in-situ bioremediation system design

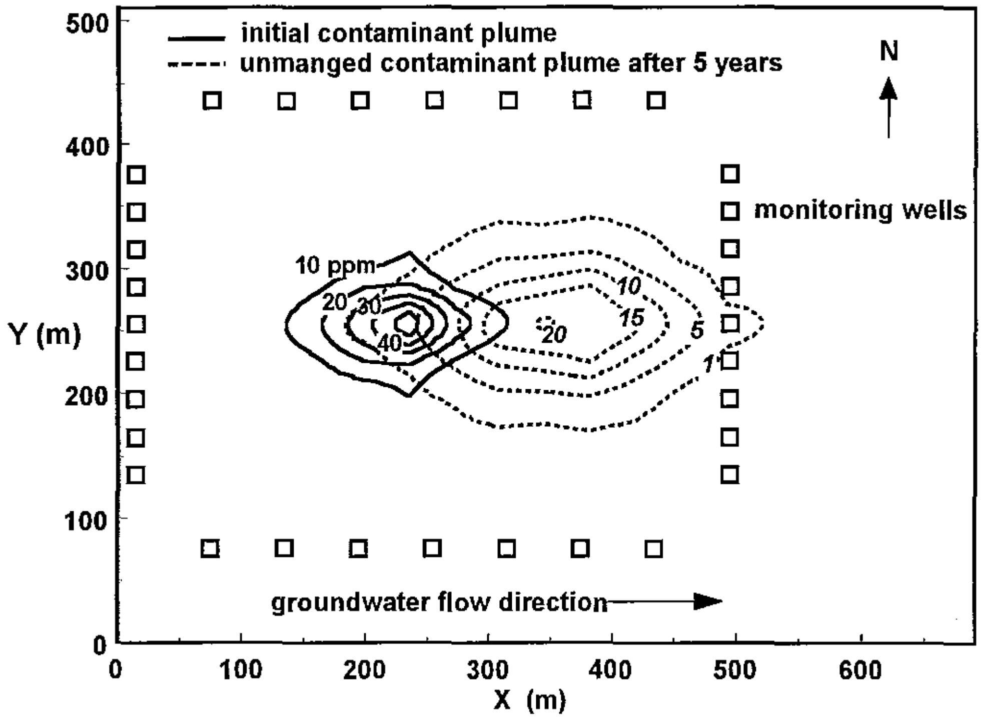

Figure 3. Initial contaminant plumes and unmanaged condition after 5 years

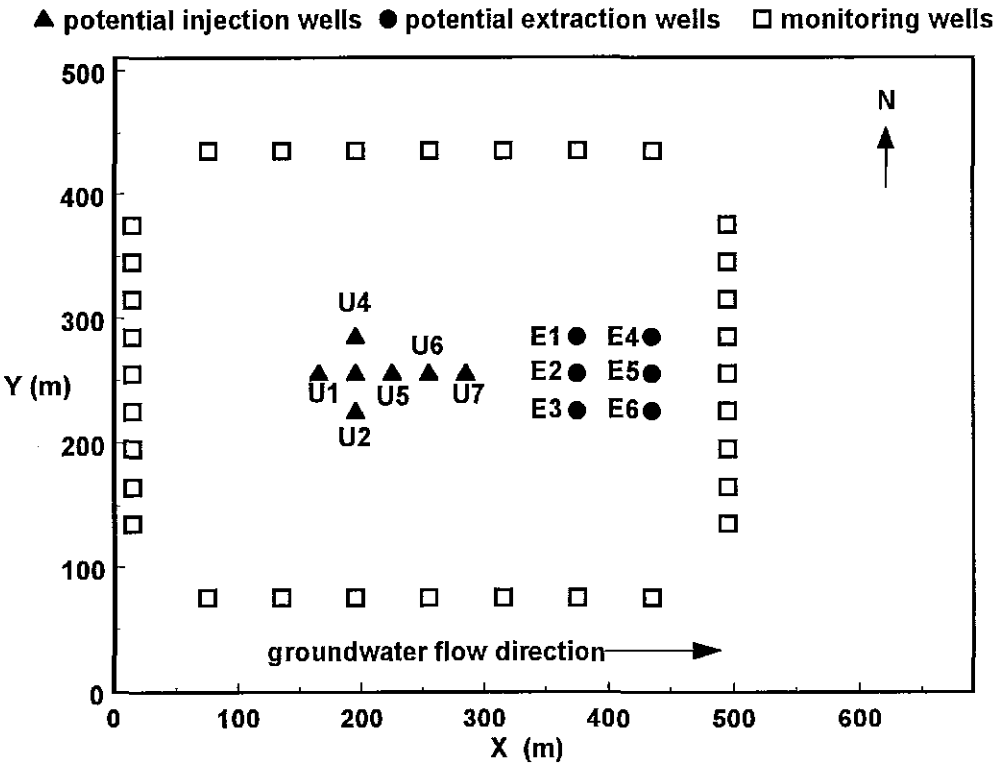

Figure 4. Proposed in-situ bioremediation system

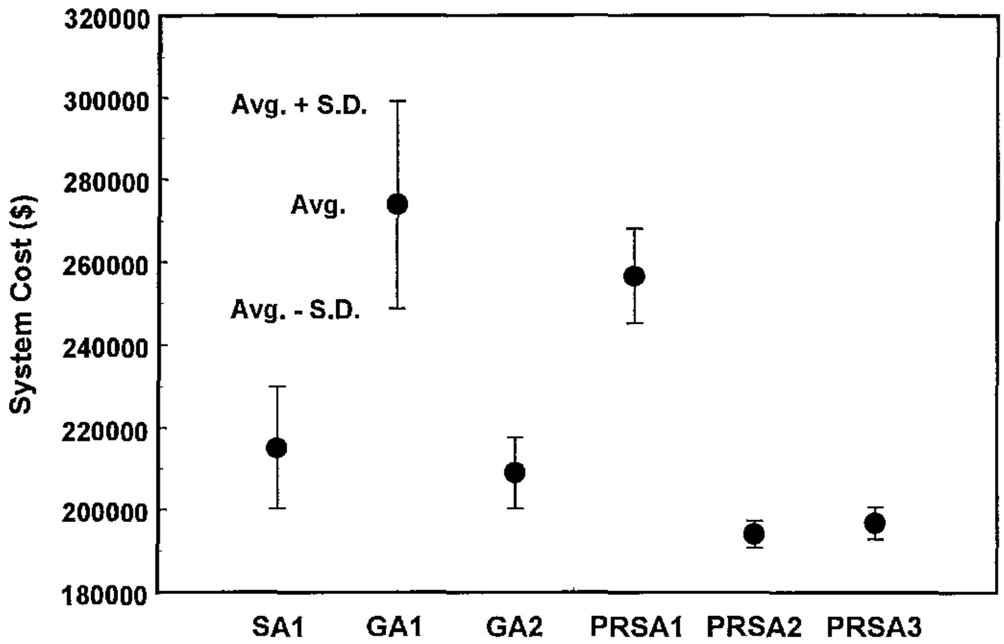

Figure 5. Error bars of SA1, GA1, GA2, PRSA1, PRSA2, and PRSA3 formulations. (Avg. = average cost and S.D. = standard deviation. Calculation of two values are based on the 20 runs)

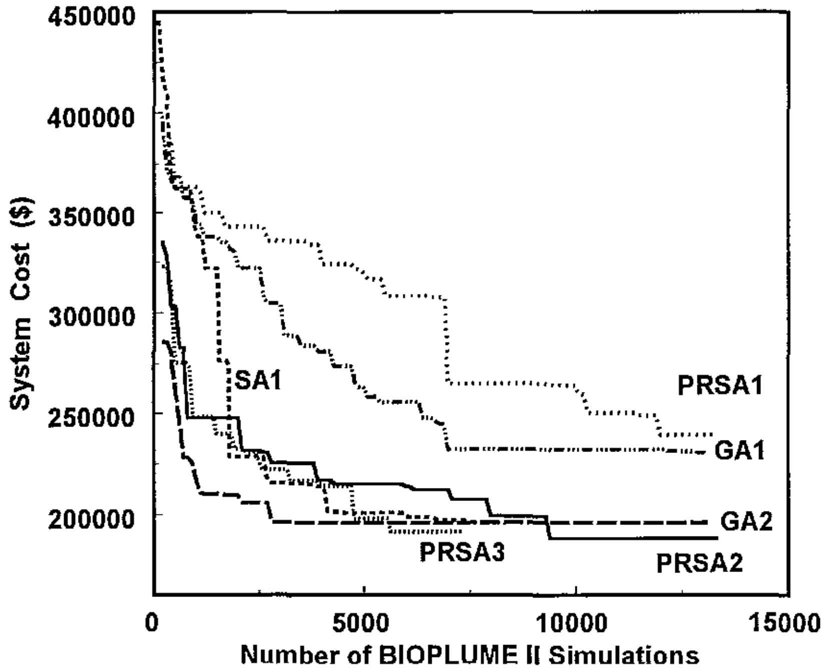

Figure 6. System cost vs. number of BIOPLUME II simulations for SA1, GA1, GA2, PRSA1, PRSA2, and PRSA3 approaches

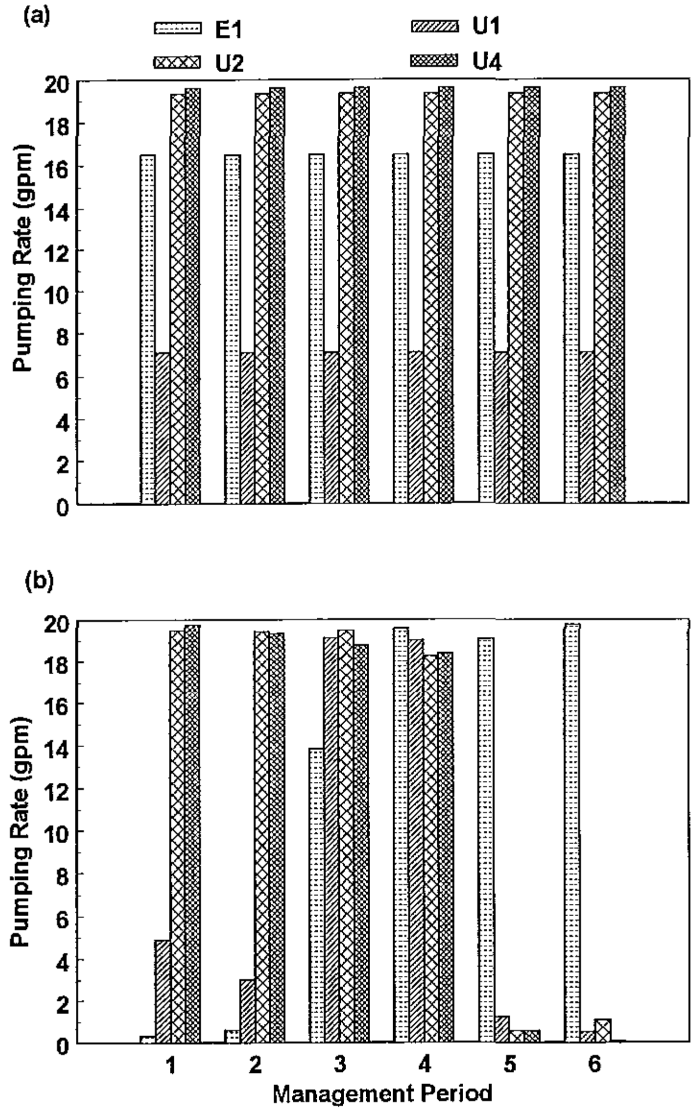

Figure 7. (a) steady pumping strategy vs. (b) time-varying pumping strategy

Rep 203

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To: "\"Richard C. Peralta\"" <peralta@cc.usu.edu>

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You can send the comments of WRR to the following address:

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or you can fax to my office fax number¡@ 886-2-2325-7474

After reviewing the comments, I will discuss with you about the resubmitting the smaller formate paper to WRR.

About the 1st paper, it is true that 'Global optimality can be theoretically proven for small nonlinear problems, but has not been proven for complex remediation problems".¡@The following references are the list of paper which applied simulated annealing (SA)¡@ to solve groundwater remediation problem. None of paper have prove that their solutions are global optimal solutions, but they all indicates that SA is a global optimizer.¡@
¡@

Dougherty, D. E. & Marryott, R. A., Optimal groundwater management: 1: Simulated annealing. Water Resources
¡@¡@¡@ Research, Vol. 27, No. 10, 1991, pp. 2493-2508.
Kuo, C.-H., Michel, A.-N. & Gray, W. G., Design of optimal pump-and-treat strategies for contaminated groundwater
¡@¡@¡@ remediation using simulated annealing algorithm. Advances in Water Resources, Vol. 15, No. 2, 1992, 95-105.

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Water Resources Research

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March 9, 1998

Dr. Richard C. Peralta
Biological and Irrigation Engineering
Utah State University
Logan, UT 84322-4105
USA

RE: WR97-605 Optimal in-situ bioremediation system design using parallel recombinative simulated annealing

Dear Dr. Peralta:

I regret to inform you that I must decline your manuscript for publication in *Water Resources Research* in its present form. However, the editors think that a new manuscript based on this work might eventually be acceptable for publication. This will probably require reducing it to the length of a Technical Note.

All three reviewers have identified the contribution of this manuscript to be the application of an algorithm (PRSA) to a problem of interest to the water resources community, namely, groundwater remediation management. You show that this algorithm can be effectively used for this problem. We think this type of contribution is best presented as a Technical Note. This could best be done by a significant reduction in the literature review and introductory material.

There is general agreement that the application of the new algorithm is technically sound. Most of the review comments address issues of clarity of presentation or value of the results. Please consider the marked manuscripts too.

The reviews are included because they should prove to be very useful in rewriting the manuscript. I encourage you to resubmit your manuscript after you undertake the major revisions suggested. However, because the required revisions are so extensive, I have decided to treat a rewritten manuscript as a new submission.

Please provide 5 copies, along with a detailed list of your responses to reviewers' comments. Your manuscript will receive a new manuscript number and will be re-reviewed. My decision to accept or to decline the manuscript will be made subsequent to that review process.

Thank you for your interest in *WRR* and we hope to hear from you in the future.

Sincerely,

Sam Colbeck
rdm

Samuel C. Colbeck
Editor

Enclosures

Additional comments of the Associate Editor on
"Optimal in-situ bioremediation system design using parallel recombinative simulated annealing"
WR97-605

1) The optimization formulation solved in this paper is described beginning on page 7. The formulation is constructed in two stages. Apparently, the well locations are selected in the first stage and the well rates and facility sizes are selected in the second stage. This method of formulation would appear to preclude the simultaneous selection of optimal well rates, locations and facility sizes. Some of the works cited by the authors have noted the importance of the well location problem in remediation design. The two stage formulation presented here may yield solutions that are not optimal relative to a formulation that allows for simultaneous selection of optimal well rates, locations and facility sizes.
   a) If the possibility of suboptimal solutions is present it should be noted in the text.
   b) The authors should explain why the formulation is constructed in this manner. Is it a requirement of the algorithm? Could other formulations also work with this algorithm? Is there some advantage to this formulation?

2) The authors state mixed integer formulations do not apply to (1). It is not clear that this is true. It appears that the problem is the staircase function defined by (2) for computing D and E in (1). Consider a formulation in which a new binary variable is defined for each of the possible states M^Q in (2). One of these new variables can be multiplied against each of the inequalities in (2). By setting these new variable to zero or one the constraint is effectively turned off or on. The formulation is completed by imposing the constraint that the sum of binary variable is 1 and that D is defined as the sum of the products of binary variables and individual capital costs. This is certainly a crude formulation - more clever ones may be available, but it appears that this problem could be formulated as a mixed integer problem.

3) The utility of Table 6 and associated text is unclear. It appears that this is an attempt to compare the current algorithm with a scheme determined by conventional engineering practice (i.e. non-optimal). This is an important comparison in concept, but is very difficult to implement. In my opinion, this can only be fruitfully done by using an algorithm on a field site where a scheme has already been designed using conventional methods. The authors should consider dropping this.

URGENT ! PLEASE RETURN REVIEW WITHIN FOUR WEEKS.

Water Resources Research's Manuscript Appraisal Form

Au .: Dr. Richard C. Peralta **Reviewer #** 1

Title: Optimal in-situ bioremediation system design using parallel recombinative simulated annealing

MS # (WR97-605)

The following questions and comments are provided as a guideline for reviewers. Please provide additional detailed comments in a written report. This form and your written report will be forwarded unedited to the author. Avoid phrasing that might generate antagonism by exaggerated, cynical, or derogatory remarks. Any confidential remarks for the editors should be included in a cover letter. Note that the paper need not agree with currently popular opinions or with your own view in order to be publishable. To serve its readership well, it is important that *WRR* provide a forum for widely diverse scientific views.

Please use either black or blue ink pens. Avoid the use of red/blue pencils on this form as these marks do not photocopy well.

1. CONTRIBUTIONS AND AUDIENCE

What are the important contributions of this paper? Introduces a new optimization method (PRSA) and contrasts its performance with that of other methods used previously for coupled simulation/optimization (S/O) in water resources management.

2. TECHNICAL SOUNDNESS

Is the paper technically sound?

Yes.

Are the methods described fully?

I suggest further elaboration on GA and PRSA methods to help clarify some sections of the paper.

Is the mathematical development complete and accurate?

N/A

3. PRIOR PUBLICATION

Has this work, or very similar work, been published elsewhere?

Plenty of coupled S/O papers have been published in WRR and elsewhere. What is new here is the optimization method.

4. ORGANIZATION AND STYLE

Is the paper well written and organized?

Generally, yes.

Are all tables and figures necessary?

Perhaps Figure 2 could be described in the text or combined with Figure 1.

Can the paper be shortened?

Not really.

5. EVALUATION

(a) Does this paper make a significant, new contribution in the area of water resources?

First use of PRSA in water resources management.

(b) How do you rate the paper?

Outstanding ____ Very Good ____ Good X Fair ____ Poor ____

Reviewer's comments for "Optimal in-situ bioremediation system design using parallel recombinative simulated annealing", by Shieh and Peralta, WR97-605.

This paper presents a coupled simulation/optimization (S/O) management model for optimizing in-situ bioremediation system design. The authors use parallel recombinative simulated annealing (PRSA) optimization combined with the BIOPLUME II simulation model. The coupled S/O model selects the appropriate combination of design variables to remediate a hypothetical contamination problem for the least cost.

The primary focus of the paper is on the optimization method, PRSA, which is a relatively new hybrid method that has not previously been applied to groundwater management problems. The simulation model is not new. Neither is the idea of incorporating bioremediation design into the S/O framework, as noted by the authors. Overall, this paper is well organized and well written and is worthy of publication in *WRR*. My comments and suggestions are provided below, as well as on the manuscript.

My major criticism concerns the description of the optimization method(s) provided on pages 11-19. Most readers will not be familiar with these methods; I suggest the following changes to help clarify the manuscript:

Page 11, paragraph 2. Expand the description of GAs **slightly** (perhaps a paragraph or two, at most). Describe the population approach, and the major operators (crossover, mutation, and selection) in more detail; some of this material appears later in the manuscript and can be removed from those sections.

Page 13, paragraph 1. It would be helpful to introduce each of the control parameters (i.e., T_0, T_f, α, N, G, etc.) at this point. How are they are selected? What are their significance?

Page 13, paragraph 3. The first part of this paragraph needs to be clarified. How are the two parent configurations chosen (randomly, sequentially) from the population? Are these parents then excluded from further operations during the current generation? How are the Boltzmann trials carried out (between which parent and child)?

Page 14, after paragraph 3. I suggest a short paragraph that explains in very general terms what Gray coding is. Briefly discuss the difference between binary coding and gray coding.

Page 15, paragraph 3. How is the explicit well installation coding different from a binary installation code assigned to each potential well location after the rates have been selected (i.e., 0 for zero pumping, 1 for non-zero pumping)? This is not clear from the text.

(1)

Page 17, paragraph 1. TAF is used twice to accept or reject the new configuration. What would be the benefit or drawback of using TAF for the first selection (to eliminate unnecessary simulation runs) and a Boltzmann trial (to allow uphill moves) for the second selection?

Page 19, description of Step 5. Are all the solutions exchanged after the current generation has been operated on, or are just the current selections exchanged? Need to clarify.

Additional comments:

Page 7, paragraph 2. I suggest using a variable other than *i* for the discount rate in the calculation of W_1, since *i* and *e* denote injection and extraction elsewhere. Also, why are W_2, W_3, and W_4 necessary if they all are equal to 1?

Page 10, paragraph 2, equation (5). Again, I suggest using a different variable for the discount rate (other than *i*). Are W_3 and W_4 here the same as those used in equation (1); are they also equal to 1?

Page 22, paragraphs 2 and 3. Why is it necessary to specify a lower bound on the hydraulic head of an injection well? Similarly, why is it necessary to specify an upper bound on the hydraulic head of an extraction well?

Page 23, paragraph 2. Where did the cost coefficients come from? Are these established from field studies? Are they hypothetical? Have they been derived from other sources (i.e., is there some reference for the coefficients)?

Page 24, paragraph 1. Values for the crossover and mutation rates should be discussed in more detail (if not here, then they should be described earlier, when crossover and mutation are originally introduced).

Page 24, paragraph 2. It would be helpful to list the six different formulations and why they were selected right from the start of this discussion.

Page 25, paragraph 2 and the discussion that follows. It is not clear which algorithms are compared in Figure 7. I assume that the second stage was conducted using PRSA, but which one (PRSA1, PRSA2, or PRSA3)? Which formulation was used for the steady pumping strategy. Please clarify.

Page 26, paragraph 3. Design B was selected based "on experience". Please elaborate on the process used to select this design configuration. Was it intentionally over-designed (i.e., more wells than necessary) just to illustrate the point? Typical "experience", especially considering the simplicity of the hypothetical example problem, would be to minimize the number of wells used in the design.

manuscript comments of reviewer 1

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

Horng-Jer Shieh and Richard C. Peralta

Biological and Irrigation Engineering Department, Utah State University

Abstract

Presented is a simulation/optimization (S/O) model combining optimization with BIOPLUME II simulation for optimizing in-situ bioremediation system design. The (S/O) model uses parallel recombinative simulated annealing to search for an optimal design and applies 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. We propose a two-stage management approach. The first stage design goal is to minimize total system cost (pumping/treatment, well installation and facility capital costs). The second stage design goal is to minimize the cost of a time-varying pumping strategy using the optimal system chosen by the first stage optimization. Optimization results show that parallel recombinative simulated annealing performs better than simulated annealing and genetic algorithms for optimizing system design when including installation costs. New explicit well installation coding improves algorithm convergence. Threshold accepting reduces

eliminating unnecessary simulation runs

computation time 43 % by rejecting expensive system designs. Applying the optimal time-varying pumping strategy in the second stage reduces pumping cost by 31%.

Key Words: in-situ bioremediation, groundwater remediation, aerobic biodegradation, optimization, parallel recombinative simulated annealing, simulated annealing, genetic algorithm.

INTRODUCTION

In-situ bioremediation for contaminated groundwater cleanup has emerged as a viable remediation technology because of cost-effectiveness and ability to achieve complete destruction of organic contaminants. Many successful applications of in-situ bioremediation for cleaning up petroleum hydrocarbons such as benzene, toluene, ethylbenzene, and xylene (BTEX) have been documented (Flathman, 1993; Hinchee et al., 1994). Major advantages of in-situ bioremediation include (1) lower capital cost, (2) in-situ operation, (3) permanent elimination of contaminants, and (4) cost-effectiveness [Cookson, 1995; Sturman et al., 1995]. An in-situ bioremediation system consists of subsurface delivery systems (injection wells, infiltration galleries or trenches) and recovery wells [Norris et al., 1994]. The recharged water provides sufficient nutrients (e.g. N and P) and electron acceptors (e.g. O_2, NO_3^{-1}, $SO4^{-2}$, Fe^{+3} and CO_2) to stimulate the growth of microorganisms that can transform the contaminants to less harmful chemicals or mineral end products [Alexander, 1994]. Downgradient recovery wells extract contaminated groundwater to contain the plume and to enhance the movement of electron acceptors and nutrients. Air stripper tower or activated carbon can treat contaminated groundwater from the recovery wells.

Taylor and Jaffe [1991] applied a bioremediation model to evaluate in-situ bioremediation design for sorbing and nonsorbing contaminants. Lang et al. [1997] designed in-situ bioremediation systems relying on cometabolic degradation. These approaches only employ bioremediation models to evaluate the efficiency of alternative system designs. It is difficult to use a simulation model alone to develop a least cost management strategy when designing a remediation system. A simulation/optimization (S/O) management model, which incorporates a groundwater flow and transport simulation model within an optimization program, can help engineers design an in-situ bioremediation system that satisfies best management goals and regulator requirements.

Many S/O applications have focused on optimal pump-and-treat (P&T) system design [Gorelick et al., 1984; Ahlfeld et al., 1988; Ahlfeld, 1990; Culver and Shoemaker, 1992; Xiang et al., 1995]. Many optimization techniques have been applied within groundwater simulation/optimization management models. Traditional optimization methods include linear programming, nonlinear programming, dynamic programming, quadratic programming, mixed-integer programming. New optimization techniques include simulated annealing [Dougherty and Marryott, 1991; Kuo et al., 1992; Marryott et al., 1993; Marryott, 1996, Rizzo and Dougherty, 1996], neural network [Rogers and Dowla, 1994; Rogers et al., 1995; Johnson and Rogers, 1995] and genetic algorithms [Ritzel et al., 1994; McKinney and Lin, 1994; Huang and Mayer, 1997]. These new techniques eliminate the requirement of computing derivatives with respect to decision variables. Such derivatives are difficult to calculate analytically or numerically in highly nonlinear and nonco n vex groundwater remediation problems. The new techniques are robust and easily coupled with groundwater simulation models.

McKinney and Lin [1994] applied genetic algorithms (GAs) to develop groundwater management strategies for goals of maximizing pumping, minimizing the cost of pumping and minimizing the cost of aquifer remediation. Their results show that genetic algorithms can obtain optimal solutions that are as good as, or better, than those solved by linear and nonlinear programming. GA advantages include straight- forward formulation and no requirement for computing derivatives. GAs using parallel programming can take advantage of network or multi-processors computers to accelerate solution convergence. However, Cieniawski et al. [1995] pointed out some shortcomings. First, ~~the~~ GAs require~~s~~ substantial CPU time for objective function evaluations. Second, ~~it~~ they handle~~s~~ multiple constraints with difficulty. Third, GAs are not theoretically guaranteed to find global optimal solutions.

Rogers and Dowla [1994] used artificial neural networks (ANNs) with parallel solute transport modeling to optimize aquifer pump-and-treat remediation. Their approach includes: (1) training an ANN to predict remediation outcome of groundwater flow and transport modelling, (2) using the trained ANN linked with a GA to search through many pumping strategies and select the one which minimizes total pumping while meeting remediation goals. In their groundwater remediation applications, Rogers et al. [1995] treated the pumping rate of each well as either 1 (full capacity pumping) or 0 (no pumping). This reduces the number of groundwater flow and transport simulations

In this study, we propose a two-stage design approach. The first stage optimizes in-situ bioremediation system configuration, including the pumping well locations, steady pumping rates and facility capacities; the objective is to minimize total system cost including pumping/treatment, well installation, and facilities capital costs. The second stage involves reducing pumping costs of the system designed in the first stage; the objective is to minimize pumping cost plus facility capital cost using a time-varying pumping strategy.

The first stage objective function is expressed as

$$\text{Minimize} \quad Z = W_1 \sum_{\hat{e}=1}^{M^p} C^p(\hat{e})\, p(\hat{e}) + W_2 \sum_{\hat{e}=1}^{M^p} C^{IP}(\hat{e})\, IP(\hat{e})$$

$$+\ W_3\, D\Big(\sum_{\hat{e}=1}^{M^i} p(\hat{e})\Big) + W_4\, E\Big(\sum_{\hat{e}=1}^{M^e} p(\hat{e})\Big) \qquad (1)$$

where Z = total present worth of in-situ bioremediation system; W_1, W_2, W_3, and W_4 are factors used to convert pumping/treatment costs, well installation costs, injection facility capital cost and treatment facility cost to their present value, respectively; $W_1 = [(1+i)^{Te}-1]/[i(1+i)^{Te}]$; i is a discount rate and Te is total duration of remediation period; W_2, W_3, and W_4 are equal to 1; ê = index denoting a potential injection or extraction location; p(ê) = injection or extraction rate at location ê (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 $\hat{e}$; $D(\sum_{\hat{e}=1}^{M^i} p(\hat{e}))$ = oxygen and nutrient injection facility capital cost, a function of total injection rate (\$); M^i = total number of injection wells; $E(\sum_{\hat{e}=1}^{M^e} p(\hat{e}))$ = treatment facility capital cost, a function of total extraction rate (\$); M^e = total number of extraction wells; and $M^p = M^i + M^e$.

Injection and treatment facilities capital cost is dependent on facility capacities. In practical engineering design, facility capital cost is not a continuous function of capacity because only specific sizes on models (or) of pipes, pumps and facilities are manufactured. Therefore, we use a discrete function to represent ~~present~~ these facility capital costs. The Capital cost of injection facility D can be expressed as

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

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

where D_q = capital cost of 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. The equation defining the capital cost of treatment facility E ~~E capital cost~~ is analogous to Eq (2) and obtained by substituting $E(\sum_{\hat{e}=1}^{M^e} p(\hat{e}))$ for

$D(\sum_{\hat{e}=1}^{M^i} p(\hat{e}))$, M^e 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.

The first management objective function is a combination of mixed-integer programming (well installation cost) and combinatorial optimization (discrete facility capacity). Traditional optimization techniques such as mixed-integer nonlinear programming cannot apply to equation (1) which is not differentiable. ~~An~~ One advantage of SA, GA and PRSA is that they do not need function derivatives.

First and second stage management model constraints include the following:

1. Upper and lower bounds on injection and extraction rates;
2. Bounds on aquifer hydraulic heads at injection and extraction wells;
3. Upper bound on final contaminant concentration needed to achieve a cleanup standard,

$$C_{k,Te} \le C_{cl} \qquad \forall k \in \Psi \tag{3}$$

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

4. Upper bound on concentration at specific locations to assure capture (prevent unacceptable concentration migration),

$$C_{o,t} \leq C_{ca} \qquad \forall o \in \Omega \tag{4}$$

t or Te as in (3)?

where $C_{o,t}$ = contaminant concentration resulting at node o by the end of period t (M/L^3); C_{ca} = maximum allowable contaminant concentration (M/L^3); and Ω = a set of monitoring wells.

In the second stage, we plan to use the wells ~~suggested for installation~~ selected by the first stage. However, in this stage we minimize the cost of injection, extraction and treat~~ing~~ment ~~water at~~ using time-varying rates. We must consider the injection and treatment facility costs since those are functions of pumping rate~~s~~. Thus, the second stage objective function is:

$$\text{Minimize} \quad U = \sum_{t=1}^{M^n}\left(\frac{1}{(1+i)^{t y_p}}\sum_{\hat{e}=1}^{M^p} C^p(\hat{e})\, p(\hat{e},t)\right)$$

$$+\ W_3\, \text{Max}\left\{D\left(\sum_{\hat{e}=1}^{M^i} p(\hat{e},t)\right)\right\}_{t=1}^{M^n} + W_4\, \text{Max}\left\{E\left(\sum_{\hat{e}=1}^{M^e} p(\hat{e},t)\right)\right\}_{t=1}^{M^n} \tag{5}$$

where U = total present worth of pumping and facility capital costs; $p(\hat{e},t)$ = injection or extraction rate at location ê for stress period t (L^3/T) (a stress period is a period of ~~unchanging~~ constant pumping); M^n = total number of stress periods; y_p = stress period duration (T). Injection and treatment facilities are constructed before enhanced bioremediation commences. Facility capital costs are determined by the capacity requirements. Injection and treatment facility capacities must not be less than the greatest total injection and extraction rates, respectively. The second phase S/O model employs the same constraints as the first phase.

PARALLEL RECOMBINATIVE SIMULATED ANNEALING

Simulated Annealing and Genetic Algorithms

The study of GAs has been well documented by many researchers [Holland, 1975; Goldberg, 1989; Davis, 1991; Michalewicz, 1992; Mitchell, 1996; Bäck, 1996; Bäck et al.,1997]. GAs 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 multireservoir operation [Oliveira and Loucks, 1997]. GAs are naturally parallel and can be easily run on networks or parallel computers. They iterate an entire population using crossover, mutation and selection operators. GAs have no formal proof of convergence to the optimal soln? and lack good control of convergence.

On the other ~~head~~ hand, SA can be mathematically proven to converge to global optimal solutions. The proof mainly depends on the annealing schedule and the Markov chain length. By slowly decreasing the 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 paralleling simulated annealing to accelerate convergence very difficult. Recently,

evolved generations, we reduce the temperature using the SA temperature update function $T_{n+1} = \alpha T_n$. As T_{n+1} decreases, uphill moves become more difficult. At low temperature, a system configuration that increases cost has little chance to win the Boltzmann trial because of low probability. The stopping criterion of PRSA is a final temperature T_f. The algorithm terminates when temperature T_f is passed.

Improvement of PRSA

New SA or GA techniques can potentially improve PRSA performance. Sample techniques are (1) Gray coding scheme, (2) explicit well installation coding, (3) uniform crossover, (4) threshold accepting function, and (5) segregated genetic algorithm.

Most GA encoding schemes use binary strings (0 and 1 bits) to represent decision variables [Holland, 1975]. Some researchers suggested real-valued coding (floating point representation) for real parameter optimization to increase efficiency and numerical precision [Wright, 1991; Goldberg, 1991; Janikow and Michalewicz, 1991; Eshelman and Schaffer, 1993; Surry and Radcliffe, 1997]. In this study, we choose Gray coding as the coding scheme of PRSA.

Gray coding can help in the following manner. Although Gray coding uses 0 and 1 bits to represent decision variables, it is an improvement because it reduces Hamming distance to 1 for adjacent decision variables. Hamming distance is defined as the number of bits difference between neighborhood substrings. The Gray code ensures that two similar solutions are represented by two similarly coded strings. Hinterding et al. [1995] found Gray code performance usually superior to binary code for function optimization.

Improvement over what

[1989] shows that uniform crossover is superior to one-point and two-point crossover theoretically and empirically. In GA water resources applications, uniform crossover applications include water distribution networks design [Savic and Walters, 1997] and multireservoir operation [Oliveira and Loucks, 1997].

Traditional GA selection operators include proportional, tournament, and ranked-based selections [Bäck et al.,1997]. However, PRSA employs a Boltzmann trial as its selection operator [Mahfound and Goldberg, 1995]. A Boltzmann trial uses the annealing temperature to control selection pressure, process? which ~~is~~ was described previously. To reduce S/O model simulation requirements, we introduce a threshold accepting function (TAF) [Dueck and Scheuer, 1990; Moscato and Fontanari, 1990; Althofer and Koschnick, 1991] to reject expensive system designs without requiring additional simulations. We will contrast the optimization results of Boltzmann trial and TAF for in-situ bioremediation system design application. in Section 6 or 7 ??

This TAF (Figure 2) uses a deterministic rule to accept or reject a new configuration. The ~~Total~~ total cost now includes the ~~total~~ system and penalty costs. The penalty cost is based on the constraints violated according to biodegradation model simulation. After the crossover and mutation operators generate a new configuration (child), we calculate $C_{child\ system}$ (child system cost) and ΔC_{system}, ($C_{parent\ system}$-$C_{child\ system}$), or the difference between parent and child system costs. If (ΔC_{system}-parent penalty cost) is larger than the current temperature T_n, the new configuration is automatically rejected. Under this condition, it is not necessary to run the simulation model because the new configuration has no chance to be accepted at the current T_n even if the new penalty cost is zero. If (ΔC_{system}-parent penalty cost) is smaller than the current T_n (i.e. new configuration reduces the system cost, or new configuration increases the system cost but has a chance to be accepted), we run the simulation model and ~~estimate a~~ calculate the child penalty cost. ΔC, (C_{parent}-C_{child}), is calculated and TAF is used again to determine whether to accept or reject the new configuration.

Constraint handling is an important issue for many design problems. Michalewicz and Schoeauer [1996] review constraint handling methods applied in evolutionary algorithms. Most of these methods employ penalty functions that penalize infeasible solutions. Here we deal with inequality constraints by expanding the objective function to include penalty cost for infeasible solutions. A penalty cost function is defined as

$$\begin{aligned} f_j(X) &= Pe(j)\, g_j(X) && \text{for violated constraint } g_j(X) > 0 \\ &= 0 && \text{for satisfied constraint } g_j(X) \le 0 \end{aligned} \qquad (6)$$

where $f_j(X)$ is a penalty cost function for j^{th} constraint ($g_j(X) \le 0$); $Pe(j)$ is a penalty coefficient for j^{th} constraint. The penalty cost is calculated by the distance from feasibility (acceptability) multiplied by a penalty cost coefficient for the violated constraint (i.e. if $g_j(X) > 0$). If the constraint is satisfied (i.e. if $g_j(X) \le 0$), the penalty cost is zero.

Specifying penalty coefficients is challenging. A high penalty coefficient will ensure most solutions lie within the feasible solution space, but can lead to costly

Step 5. Exchange individual solutions between the new large penalty and small penalty parent populations.

Step 6. Continue step 2 through step 5 until stopping criterion is satisfied.

GROUNDWATER BIODEGRADATION MODELS

Computer models incorporating microbial growth and biodegradable pollutant~~s~~ transport can be classified according to conceptual approach [Baveye and Valocchi, 1989]. The first approach, which has been applied to biological wastewater treatment, uses a biofilm concept to simulate trace-organics biodegradation in the subsurface [Rittmann et al., 1980]. The second approach assumes contaminant transport and biodegradation occur in small discrete colonies attached to the surface of the solid aquifer particles [Molz et al., 1986]. They assume that a microcolony has the form of a cylindrical plate with a radius and thickness and can be viewed as a simplified biofilm model. The third approach is strictly macroscopic and makes no assumption about microorganism distribution within the pore space. Removal of organic contaminant is assumed to be by Monod or Michaelis-Menten kinetics involving aerobic degradation and anaerobic degradation in the subsurface [Borden and Bedient, 1986]. A simplified simulation model using the third approach, BIOPLUME II, assumes that aerobic biodegradation can be treated as an instantaneous reaction [Rifai et al., 1988; Rifai and Bedient, 1990].

The BIOPLUME II model uses a dual-particle mover procedure to simulate subsurface oxygen and contaminant~~s~~ transport. It was developed by modifying a two-

$$\Delta C_{RO} = CF \; ; \quad C = 0 \quad \text{if} \quad O > CF \tag{10}$$

where ΔC_{RC} and ΔC_{RO} = calculated change in contaminant and oxygen concentrations, respectively; F = ratio of consumed oxygen to consumed contaminant.

BIOPLUME II can be calibrated and applied using data such as hydrogeological parameters, contaminant chemical and physical properties, contaminant source concentrations, and background oxygen concentration. Limitations of the BIOPLUME II model are : (1) it is unsuitable for simulating slowly biodegraded contaminants under aerobic conditions because of its instantaneous reaction assumption, and (2) it is incapable of simulating anaerobic processes affected by other electron acceptors such as nitrate, ferric iron, sulfate and inorganic carbon. Here we use BIOPLUME II to simulate aerobic biodegradation processes and contaminant transport within a simulation/optimization management model.

STUDY CASE

Figure 3 illustrates the hypothetical study area and the initial contaminant plume. Table 1 presents BIOPLUME II input parameters for the 510 m by 690 m study area. The homogeneous aquifer has a hydraulic conductivity of 6×10^{-5} m/sec and a thickness of 15 m ~~aquifer thickness~~. To the West and East are fixed head boundaries -- 30.5 and 27.7 m, respectively. Groundwater flow is from West to East. The initial hydraulic gradient is 0.004. To the North and South are no-flow boundaries. Groundwater flow simulation is steady state. The contaminant retardation factor is assumed to be 1.

Figure 3 illustrates the plume configuration after 5 years if no action is taken. It will move and expand, reaching the monitoring wells. Natural aerobic decay reduces the total contaminant mass by only 16 %. An in-situ bioremediation system should be installed to contain the contaminant plume and enhance contaminant biodegradation.

To design an in-situ bioremediation system, the optimization will consider potential injection and extraction wells. Seven wells within the plume can potentially inject water containing oxygen and nutrients at rates between 0 and 20 gpm (1.26 liter/sec). Upper and lower bounds ~~of~~ on hydraulic head for the injection wells are 33.5 and 27.7 m, respectively. The initial oxygen concentration is 5 ppm except in the contaminant plume area, where the oxygen concentrations have been consumed by aerobic biodegradation. The vertical exchange of oxygen with the unsaturated zone is assumed to be insignificant. The injected oxygen concentration is 8 ppm. BIOPLUME II model assumes that injected water provides enough nutrients to support microbial growth in the aquifer.

Figure 4 illustrates the potential well locations considered by the optimization. Six downgradient wells can potentially extract contaminated groundwater at rates between 0 and 20 gpm. The upper and lower bounds ~~of~~ on hydraulic head for the extraction wells are 30.5 and 24.4 m, respectively. The cleanup standard, C_{cl} , is 3 ppm for the entire study area.

Figure 4 also identifies monitoring wells (not subject to optimization) used to observe whether the plume is captured during a three-year remediation period. Because the system can inject potentially much water, additional monitoring wells are installed in

the Western boundary. This helps ensure that unacceptable plume spreading does not result. The maximum contaminant concentration allowed to reach monitoring wells, C_{ca} , is 1 ppm.

Table 2 lists the cost coefficients used to estimate system costs. The injection coefficient is based on the nutrient~~s~~, oxygen and pumping operation costs. The extraction cost coefficient considers the cost of treating and pumping contaminated groundwater. Treatment includes air stripping and granular activated carbon. Injection and treatment facilities capital costs are based on their capacities.

APPLICATIONS AND RESULTS

Optimal In-situ Bioremediation System Design with Fixed Cost

The first stage management goal is to minimize the total system cost which includes pumping/treatment, well installation, and facilities capital costs. Below we contrast the abilities of SA ,GA and PRSA ~~varieties~~ algorithms to achieve this goal. In SA we use a threshold accepting function and Corana's neighborhood search [Corana et al., 1987] to reduce SA computation cost and extend its ability to deal with continuous variables. Our two GA formulations are based on the methodology of McKinney and Lin [1994], but include replacing binary code with Gray code and the use of uniform crossover. Our GAs also extend the tournament size of tournament selection from 2 to 4 to increase selection intensity [Blickle and Thiele, 1996] and to improve convergence. We implement segregated GA to refine search in both feasible and infeasible regions. The parameter choice of GAs and PRSA is problem-dependent. After some test runs, we choose a population size of 100 for optimizing system design with fixed cost and 200 for minimizing the cost of time-varying pumping strategy. Crossover and mutation rates used for GAs and PRSA are 0.9 - 1.0 and 0.01 - 0.03, respectively.

We use six formulations to compare the three optimization algorithms. Because of the stochastic nature of these algorithms, we run each formulation twenty times using different random seeds. Table 3 lists maximum, minimum and average system costs of these runs for the six formulations. Figure 5 illustrates the error bars of the six formulations. The upper and lower caps indicate the average system cost plus or minus one standard deviation, respectively. ~~The~~ A large standard deviation reflects that the optimization algorithm does not converge to the same optimal solution consistently.

PRSA2 (PRSA with Boltzmann trial and explicit well installation) designs the least-cost system ($188,6 00). It also has the lowest average system cost ($193,900) and the smallest standard deviation (Figure 5). GA2 and PRSA2 perform well because of explicit well installation coding. GA1 and PRSA1 using implicit well installation do not converge to optimal solutions. It is difficult for GA1 and PRSA1 to reduce well numbers because implicit well installation depends on whether or not pumping rates reach zero. SA1 shows that SA can converge to optimal solutions but is not as stable as PRSA (note the large standard deviation in Figure 5). Threshold accepting helps SA1 and PRSA3 converge to optimal solution using fewer simulations. For example, PRSA3 reduces the average number of simulations by 43% compared with PRSA2, while still maintaining reasonably good solution quality (low average system cost and small standard deviation).

URGENT ! PLEASE RETURN REVIEW WITHIN FOUR WEEKS.

Water Resources Research's Manuscript Appraisal Form

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Title: Optimal in-situ bioremediation system design using parallel recombinative simulated annealing

MS # (WR97-605)

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1. CONTRIBUTIONS AND AUDIENCE

What are the important contributions of this paper?

Presents a new algorithm for the optimization of bioremediation systems.

2. TECHNICAL SOUNDNESS

Is the paper technically sound?

Yes

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Is the mathematical development complete and accurate?

Yes

3. PRIOR PUBLICATION

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No

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Is the paper well written and organized?

Yes

Are all tables and figures necessary?

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Can the paper be shortened?

No

5. EVALUATION

(a) Does this paper make a significant, new contribution <u>in the area of water resources</u>?

~~B~~ Yes, in the area of algorithm development.

(b) How do you rate the paper?

Outstanding ____ Very Good ____ Good X Fair ____ Poor ____

2

RE: WR97-605 Optimal in-situ bioremediation system design using PRSA

In general the paper is very well written and presents an application of a relatively new hybrid optimization approach, parallel recombinative simulated annealing (PRSA) to determine effective systems for remediating an aquifer by biological agents. The hypothetical application of the method is very standard and has been studied by several other researchers. The methodology applied to model the biodegradation of contaminants in the aquifer is standard and does not present new material to the literature or the readership of WRR. The contribution of this paper is in the application of PRSA, a relatively new and effective combination of genetic algorithm and simulated annealing optimization methods, to the remediation problem. Therefore, I recommend that the paper be published in WRR.

My specific comments can be found marked on the manuscript.

WR97-605
#2

manuscript review comments by reviewer 2

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

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Biological and Irrigation Engineering Department, Utah State University

Abstract

Presented is a simulation/optimization (S/O) model combining optimization with BIOPLUME II ~~simulation~~ for optimizing in-situ bioremediation system design. The (S/O) model uses parallel recombinative simulated annealing to search for an optimal design and applies 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. We propose a two-stage management approach. The first stage design goal is to minimize total system cost (pumping/treatment, well installation and facility capital costs). The second stage design goal is to minimize cost of a time-varying pumping strategy using the optimal system chosen by the first stage optimization. Optimization results show that parallel recombinative simulated annealing performs better than simulated annealing and genetic algorithms for optimizing system design when including installation costs. New explicit well installation coding improves algorithm convergence. Threshold accepting reduces

computation time 43 % by rejecting expensive system designs. Applying the optimal time-varying pumping strategy in the second stage reduces pumping cost by 31%.

Key Words: in-situ bioremediation, groundwater remediation, aerobic biodegradation, optimization, parallel recombinative simulated annealing, simulated annealing, genetic algorithm.

INTRODUCTION

In-situ bioremediation for contaminated groundwater cleanup has emerged as a viable remediation technology because of its cost-effectiveness and ability to achieve complete destruction of organic contaminants. Many successful applications of in-situ bioremediation for cleaning up petroleum hydrocarbons such as benzene, toluene, ethylbenzene, and xylene (BTEX) have been documented (Flathman, 1993; Hinchee et al., 1994). Major advantages of in-situ bioremediation include (1) lower capital cost, (2) in-situ operation, (3) permanent elimination of contaminants, and (4) cost-effectiveness [Cookson, 1995; Sturman et al., 1995]. An in-situ bioremediation system consists of subsurface delivery systems (injection wells, infiltration galleries or trenches) and recovery wells [Norris et al., 1994]. The recharged water provides sufficient nutrients (e.g. N and P) and electron acceptors (e.g. O_2, NO_3^{-1}, $SO4^{-2}$, Fe^{+3} and CO_2) to stimulate the growth of microorganisms that can transform the contaminants to less harmful chemicals or mineral end products [Alexander, 1994]. Downgradient recovery wells extract contaminated groundwater to contain the plume and to enhance movement of

lower than what?

what's the difference between 1+4?

surface treatment and chemical mixing system electron acceptors and nutrients. Air stripp~~er~~ing towers or activated carbon can treat contaminated groundwater from the recovery wells.

Taylor and Jaffe [1991] applied a bioremediation model to evaluate in-situ bioremediation design for sorbing and nonsorbing contaminants. Lang et al. [1997] designed in-situ bioremediation systems relying on cometabolic degradation. These approaches only employ bioremediation models to evaluate the efficiency of alternative system designs. It is difficult to use a simulation model alone to develop a least cost management strategy when designing a remediation system. A simulation/optimization (S/O) management model, which incorporates a groundwater flow and transport simulation model with an optimization program, can help engineers design an in-situ bioremediation system that satisfies best management goals and regulatory requirements.

Many S/O applications have focused on ~~optimal~~ optimizing pump-and-treat (P&T) system design [Gorelick et al., 1984; Ahlfeld et al., 1988; Ahlfeld, 1990; Culver and Shoemaker, 1992; Xiang et al., 1995]. Many optimization techniques have been applied within groundwater simulation/optimization management models. Traditional optimization methods include linear programming, nonlinear programming, dynamic programming, quadratic programming, and mixed-integer programming. New optimization techniques include simulated annealing [Dougherty and Marryott, 1991; Kuo et al., 1992; Marryott et al., 1993; Marryott, 1996, Rizzo and Dougherty, 1996], neural networks [Rogers and Dowla, 1994; Rogers et al., 1995; Johnson and Rogers, 1995] and genetic algorithms [Ritzel et al., 1994; McKinney and Lin, 1994; Huang and Mayer, 1997]. These new techniques eliminate the requirement of computing derivatives with respect to decision variables. Such derivatives are difficult to calculate analytically or numerically in highly nonlinear and noncovex groundwater remediation problems. The new techniques are robust and easily coupled with groundwater simulation models.

McKinney and Lin [1994] applied genetic algorithms (GAs) to develop groundwater management strategies for goals of maximizing pumping, minimizing cost of pumping and minimizing cost of aquifer remediation. Their results show that genetic algorithms can obtain optimal solutions that are as good as or better than those solved by linear and nonlinear programming. GA advantages include straight- forward formulation and no requirement for computing derivatives. GAs using parallel programming can take advantage of network or multi-processor~~s~~ computers to accelerate solution convergence. However, Cieniawski et al. [1995] pointed out some shortcomings. First, the GA requires substantial CPU time for objective function evaluations. Second, it handles multiple constraints with difficulty. Third, GAs are not theoretically guaranteed to find global optimal solutions.

Rogers and Dowla [1994] used artificial neural networks (ANNs) with parallel solute transport modeling to optimize aquifer pump-and-treat remediation. Their approach includes: (1) training an ANN to predict remediation outcome of groundwater flow and transport modelling, and (2) using the trained ANN linked with a GA to search through many pumping strategies and select the one which minimizes total pumping while meeting remediation goals. In their groundwater remediation applications, Rogers et al. [1995] treated the pumping rate of each well as either 1 (full capacity pumping) or 0 (no pumping). This reduces the number of groundwater flow and transport simulations needed to train an ANN to predict remediation outcome, but is impractical for real-world applications. Rogers and Dowla [1994] planned to apply ANNs to deal with continuous pumping. However, the computation efficiency and ability of ANNs to find optimal solutions for continuous pumping problems are still unknown.

Dougherty and Marryott [1991] first apply simulated annealing (SA) to groundwater management problems. Marryott [1996] optimizes groundwater remediation design of an interceptor trench, slurry wall and low permeability cap using SA. Those SA groundwater management applications assume a discrete solution space. Pumping rates ~~were~~ are treated as discrete decision variables. SA has advantages similar to GA. SA is easily implemented with groundwater simulation models and does not require derivative computation. In addition, SA convergence to globally optimal solutions has been proven using homogeneous Markov chain and inhomogeneous Markov chain theory [Geman and Geman, 1984; Hajek, 1988; Romeo, F. and A. Sangiovanni-Vincentelli, 1991]. Because SA sequentially searches for an optimal solution, applying parallel programming to accelerate convergence speed is more difficult with SA than with GA.

We propose applying a new optimization algorithm, parallel recombinative simulated annealing (PRSA), to optimize in-situ bioremediation system design. Mahfound and Goldberg [1995] introduced PRSA as an effective combination of SA and GA~~s~~. PRSA retains the desirable asymptotic convergence of SA and adds the GA's population approach and recombinative operator. Here, we present the first application of PRSA to in-situ bioremediation or groundwater management system design. The manuscript is organized as follows. In section 2, we formulate the management problem and describe the two-stage management approach. In section 3, we provide an overview of PRSA and its implementation. We also propose new techniques to improve PRSA performance. These techniques include Gray coding, uniform crossover, threshold accepting function and segregated genetic algorithm. In sections 4 and 5, we briefly introduce the bioremediation simulation model and describe the system design study case. In sections 6 and 7, we demonstrate in-situ bioremediation system design by PRSA and summarize findings.

OPTIMAL SYSTEM DESIGN OF IN-SITU BIOREMEDIATION

Minsker and Shoemaker [1996] proposed dynamic optimal control via successive approximation linear quadratic regulator (SALQR), to optimize in-situ bioremediation design. Their optimal time-varying pumping strategy reduced the cost of in-situ bioremediation by 30 % compared with a steady pumping strategy during two-year cleanups [Minsker, 1995]. Their cost function considered pumping operation, maintenance, oxygen addition, and treatment costs. It did not include well installation and facilities capital costs – costs which can dominate in-situ bioremediation or P&T system costs for a short remediation period. Culver and Shoemaker [1997] demonstrate that capital treatment costs significantly affect a time-varying 5-year P&T pumping strategy period. They recommend explicitly incorporating these capital costs into a dynamic management model.

Doesn't pumping rate affect capital cost through the number of wells installed?

In this study, we propose a two-stage design approach. The first stage optimizes in-situ bioremediation system configuration, including the pumping well locations, steady pumping rates and facility capacities; the objective is to minimize total system cost including pumping/treatment, well installation, and facilities capital costs. The second stage involves reducing pumping costs of the system designed in the first stage; the objective is minimize pumping cost plus facility capital cost using a time-varying pumping strategy.

The first stage objective function is expressed as

$$\text{Minimize} \quad Z = W_1 \sum_{\hat{e}=1}^{M^p} C^p(\hat{e})\, p(\hat{e}) + W_2 \sum_{\hat{e}=1}^{M^p} C^{IP}(\hat{e})\, IP(\hat{e})$$

$$+\ W_3\, D\Big(\sum_{\hat{e}=1}^{M^i} p(\hat{e})\Big) + W_4\, E\Big(\sum_{\hat{e}=1}^{M^e} p(\hat{e})\Big) \qquad (1)$$

where Z = total present worth of in-situ bioremediation system; W_1, W_2, W_3, and W_4 are factors used to convert pumping/treatment costs, well installation costs, injection facility capital cost and treatment facility cost to their present value, respectively; $W_1 = [(1+i)^{Te}-1]/[i(1+i)^{Te}]$; i is a discount rate and Te is total duration of remediation period; W_2, W_3, and W_4 are equal to 1; $\hat{e}$ = 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 $\hat{e}$; $D(\sum_{\hat{e}=1}^{M^i} p(\hat{e}))$ = oxygen and nutrient injection facility capital cost, a function of total injection rate ($); M^i = total number of injection wells; $E(\sum_{\hat{e}=1}^{M^e} p(\hat{e}))$ = treatment facility capital cost, a function of total extraction rate ($); M^e = total number of extraction wells; and $M^p = M^i + M^e$.

Injection and treatment facilities capital cost is dependent on facility capacities. In practical engineering design, facility capital cost is not a continuous function of capacity because only specific sizes on models of pipes, pumps and facilities are manufactured. Therefore, we use discrete function s to present these facility capital costs. The ~~C~~apital cost of injection facility D can be expressed as

$$
\begin{aligned}
D\left(\sum_{\hat{e}=1}^{M^i} p(\hat{e})\right) &= 0 \quad \text{if} \quad \sum_{\hat{e}=1}^{M^i} p(\hat{e}) = 0 \\
&= D_q \quad \text{if} \quad CD_{q-1} < \sum_{\hat{e}=1}^{M^i} p(\hat{e}) \le CD_q \quad q = 1, 2, \ldots\ldots, M^Q
\end{aligned}
\tag{2}
$$

where D_q = capital cost of injection facility when total injection rate is between design injection capacity CD_{q-1} and CD_q; and M^Q is the total number of alternative design injection capacities. Injection capacity CD_0 is 0. The equation defining treatment facility E capital cost is analogous to Eq (2) and obtained by substituting $E(\sum_{\hat{e}=1}^{M^e} p(\hat{e}))$ for

D($\sum_{\hat{e}=1}^{M^{i}} p(\hat{e})$), M^e 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 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.

The first management objective function is a combination of mixed-integer programming (well installation cost) and combinatorial optimization (discrete facility capacity). Traditional optimization techniques such as mixed-integer nonlinear programming cannot apply to equation (1) which is not differentiable. An advantage of SA, GA and PRSA is they do not need function derivatives

First and second stage management model constraints include the following:

1. Upper and lower bounds on injection and extraction rates
2. Bounds on aquifer hydraulic heads at injection and extraction wells
3. Upper bound on final contaminant concentration needed to achieve a cleanup standard

$$C_{k,\,Te} \le C_{cl} \qquad \forall k \in \Psi \tag{3}$$

where $C_{k,Te}$ = contaminant concentration at node k by the end of time period Te (M/L^3); C_{cl} = 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 study area nodes.

commences. Facility capital costs are determined by the capacity requirement. Injection and treatment facility capacities must not be less than the greatest total injection and extraction rates, respectively. The second phase S/O model employs the same constraints as the first phase.

PARALLEL RECOMBINATIVE SIMULATED ANNEALING

Simulated Annealing and Genetic Algorithms

The study of GAs has been well documented by many researchers [Holland, 1975; Goldberg, 1989; Davis, 1991; Michalewicz, 1992; Mitchell, 1996; Bäck, 1996; Bäck et al.,1997]. GAs have been applied to many water resources management problems such as pipe networks [Simpson et al., 1994; Dandy et al., 1996], groundwater remediation [Ritzel et al., 1994; McKinney and Lin, 1994] and multireservoir operation [Oliveira and Loucks, 1997]. GAs are naturally parallel and can be easily run on networks or parallel computers. They iterate an entire population using crossover, mutation and selection operators. GAs have no formal proof of convergence and lack good control of convergence.

On the other ~~head,~~ hand SA can be mathematically proven to converge to global optimal solutions. The proof mainly depends on the annealing schedule. By slowly decreasing the 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 paralleling simulated annealing to accelerate convergence very difficult. Recently, researchers have investigated hybrid genetic annealing algorithm (GAA) approaches that combine desirable attributes of GA and SA methods [Sirag and Weisser, 1987; Brown et al., 1989; Boseniuk and Ebeling, 1991; Lin et al., 1993; Chen and Flann, 1994; Mahfound and Goldberg, 1995; Yong et al., 1995; Varanelli and Cohoon, 1995; Jeong and Lee, 1996]. The intended result is a general-purpose optimization algorithm that has the good SA convergence control and the efficient GA parallelization. Chen and Flan [1994] investigated 14 hybrid methods of combining GA and SA. For nine optimization problems, combining GA crossover and mutation operators with SA annealing schedule ~~has~~ yielded the best performance. Varanelli and Cohoon [1995] used population-oriented simulated annealing (POSA) to solve a VLSI network partitioning problem. Their results showed that POSA converged to a better optimal solution than GA for the same CPU time.

Goldberg [1990] introduced the annealing schedule and the Boltzmann distribution to help prove GA convergence to global optimality. Mahfound and Goldberg [1995] presented a parallel recombinative simulated annealing (PRSA) algorithm and proved its asymptotic global convergence. For their test problems, PRSA consistently converged to the global optimum. The PRSA algorithm effectively combines simulated annealing and genetic algorithms to offer the user control over convergence.

evolved generations, we reduce the temperature using the SA temperature update function $T_{n+1} = \alpha T_n$. As T_{n+1} decreases, uphill moves become more difficult. At low temperature, a system configuration that increases cost has little chance to win the Boltzmann trial because of low probability. The stopping criterion of PRSA is a final temperature T_f. The algorithm terminates when temperature T_f is passed.

Improvement of PRSA

New SA or GA techniques can potentially improve PRSA performance. Sample techniques are (1) Gray coding scheme, (2) explicit well installation coding, (3) uniform crossover, (4) threshold accepting function, and (5) segregated genetic algorithm.

Most GA encoding schemes use binary strings (0 and 1 bits) to represent decision variables [Holland, 1975]. Some researchers suggested real-valued coding (floating point representation) for real parameter optimization to increase efficiency and numerical precision [Wright, 1991; Goldberg, 1991; Janikow and Michalewicz, 1991; Eshelman and Schaffer, 1993; Surry and Radcliffe, 1997]. In this study, we choose Gray coding as the coding scheme of PRSA.

Gray coding can help in the following manner. Although Gray coding uses 0 and 1 bits to represent decision variables, it is an improvement because it reduces Hamming distance to 1 for adjacent decision variables. Hamming distance is defined as the number of bits difference between neighborhood substrings. The Gray code ensures that two similar solutions are represented by two similarly coded strings. Hinterding et al. [1995] found Gray code performance usually superior to binary code for function optimization.

Dandy et al. [1996] use Gray code to improve GA performance for pipe network optimization. Rana and Whitley [1997] prefer Gray coding for bit representation in GA.

In groundwater remediation design involving well installation, installation cost is usually treated as an implicit decision variable such that well installation cost is zero if pumping rate is zero or close to zero [McKinney and Lin, 1995; Sawyer and Ahlfeld, 1995]. Huang and Mayer [1997] use well locations as explicit decision variables in P&T GA optimization. They encode the x and y coordinates of well locations into a GA substring. Their objective is to minimize P&T cost by optimizing well locations and pumping rates simultaneously, but well installation cost is still determined by pumping rate (i.e. no well installation if pumping rate is zero).

Here we propose a new approach which we ~~termed~~ explicit well installation coding. Each pumping well installation is explicitly coded as 1 or 0 bit values representing whether the well is or is not installed, respectively. Initially, PRSA randomly generates system configurations indicating injection and extraction well installation. Using crossover, mutation, and Boltzmann trial, PRSA optimizes the number of installed pumping wells and pumping rates to minimize system cost.

Crossover, mutation and selection are three important GA operators. Two parent solutions use crossover and mutation to create two child solutions. Then, the selection operator selects solutions from the current population to form the next evolved generation. Mutation is usually a background operator in GA. The two main operators are crossover and selection. Traditional crossover operators are one-point and two-point crossover [Goldberg, 1989]. We choose uniform crossover for PRSA because Syswerda

[1989] shows that uniform crossover is superior to one-point and two-point crossover theoretically and empirically. In GA water resources applications, uniform crossover applications include water distribution networks design [Savic and Walters, 1997] and multireservoir operation [Oliveira and Loucks, 1997].

Traditional GA selection operators include proportional, tournament, and ranked-based selections [Bäck et al.,1997]. However, PRSA employs Boltzmann trial as its selection operator [Mahfound and Goldberg, 1995]. A Boltzmann trial uses annealing temperature to control selection pressure, which is described previously. To reduce S/O model simulation requirements, we introduce a threshold accepting function (TAF) [Dueck and Scheuer, 1990; Moscato and Fontanari, 1990; Althofer and Koschnick, 1991] to reject expensive system design without requiring additional simulations. We will contrast the optimization results of Boltzmann trial and TAF for in-situ bioremediation system design application.

This TAF (Figure 2) uses a deterministic rule to accept or reject a new configuration. Total cost now includes total system and penalty costs. The penalty cost is based on constraints violated according to biodegradation model simulation. After the crossover and mutation operators generate a new configuration (child), we calculate $C_{child\ system}$ (child system cost) and ΔC_{system}, ($C_{parent\ system}$-$C_{child\ system}$), or the difference between parent and child system costs. If (ΔC_{system}-parent penalty cost) is larger than the current temperature T_n, the new configuration is automatically rejected. Under this condition, it is not necessary to run the simulation model because the new configuration conservative system designs. A low penalty coefficient permits searching both feasible and infeasible regions, but can cause convergence to an infeasible system design.

Le Riche et al. [1995] introduce a segregated genetic algorithm to reduce penalty weight influence. The segregated GA uses two penalty coefficient values instead of one. It maintains two populations: individuals selected from a large penalty population will more likely stay in the feasible region; individuals selected from a small penalty population will probably remain in the infeasible region. Eventually, the optimization algorithm will converge to the feasible optimum from both sides of the feasible region boundary. We adapted this segregated method to PRSA procedures:

Step 1. Generate two parent populations randomly. Evaluate the objective function values of one population using large penalty coefficients. Evaluate the other population using small penalty coefficients.

Step 2. Each parent population uses crossover and mutation to generate its child population.

Step 3. Evaluate the objective function values of the child population of the large penalty parent population using large penalty coefficients. Evaluate the objective function values of the child population of small penalty parent population using the small penalty coefficients.

Step 4. the New large penalty parent population is selected by competition between the current large penalty parent and child populations using Boltzmann trial or TAF. the ~~N~~ew small penalty parent population is selected by the competition between the current small penalty parent and child populations using Boltzmann trial or TAF.

Step 5. Exchange individual solutions between the new large penalty and small penalty parent populations.

Step 6. Continue step 2 through step 5 until stopping criterion is satisfied.

GROUNDWATER BIODEGRADATION MODELS

Computer models incorporating microbial growth and biodegradable pollutant~~s~~ transport can be classified according to conceptual approach [Baveye and Valocchi, 1989]. The first approach, which has been applied to biological wastewater treatment, uses a biofilm concept to simulate trace-organics biodegradation in the subsurface [Rittmann et al., 1980]. The second approach assumes contaminant transport and biodegradation occur in small discrete colonies attached to the surface of the solid aquifer particles [Molz et al., 1986]. the second approach ~~They~~ assume that a microcolony has the form of a cylindrical plate with radius and thickness and can be viewed as a simplified biofilm model. The third approach is strictly macroscopic and makes no assumption about microorganism distribution within the pore space. Removal of organic contaminant is assumed to be by Monod or Michaelis-Menten kinetics involving aerobic degradation and anaerobic degradation in the subsurface [Borden and Bedient, 1986]. A simplified simulation model using the third approach, BIOPLUME II, assumes that aerobic biodegradation can be treated as an instantaneous reaction [Rifai et al., 1988; Rifai and Bedient, 1990].

The BIOPLUME II model uses a dual-particle mover procedure to simulate subsurface oxygen and contaminant~~s~~ transport. It was developed by modifying a two-

$$\Delta C_{RO} = CF \;; \quad C = 0 \quad \text{if} \quad O > CF \qquad (10)$$

where ΔC_{RC} and ΔC_{RO} = calculated change in contaminant and oxygen concentrations, respectively; F = ratio of consumed oxygen to consumed contaminant.

BIOPLUME II can be calibrated and applied using data such as hydrogeological parameters, contaminant chemical and physical properties, contaminant source concentrations, and background oxygen concentration. Limitations of the BIOPLUME II model are : (1) it is unsuitable for simulating slowly biodegraded contaminants under aerobic conditions because of its instantaneous reaction assumption, and (2) it is incapable of simulating anaerobic processes ~~affected by~~ utilizing other electron acceptors such as nitrate, ferric iron, sulfate and inorganic carbon. Here we use BIOPLUME II to simulate aerobic biodegradation processes and contaminant transport within a simulation/optimization management model.

STUDY CASE

Figure 3 illustrates the hypothetical study area and the initial contaminant plume. Table 1 presents BIOPLUME II input parameters for the 510 m by 690 m study area. The homogeneous aquifer has a hydraulic conductivity 6 x 10^{-5} m/sec and a 15 m aquifer thickness. To the West and East are fixed head boundaries -- 30.5 and 27.7 m, respectively. Groundwater flow is from West to East. The initial hydraulic gradient is 0.004. To the North and South are no-flow boundaries. Groundwater flow simulation is steady state. The contaminant retardation factor is assumed to be 1.

Figure 3 illustrates the plume configuration after 5 years if no action is taken. It will move and expand, reaching the monitoring wells. Natural aerobic decay reduces the total contaminant mass by only 16 %. An in-situ bioremediation system should be installed to contain the contaminant plume and enhance contaminant biodegradation.

To design an in-situ bioremediation system, the optimization will consider potential injection and extraction wells. Seven wells within the plume can potentially inject water containing oxygen and nutrients at rates between 0 and 20 gpm (1.26 liter/sec). Upper and lower bounds of hydraulic head for the injection wells are 33.5 and 27.7 m, respectively. The initial oxygen concentration is 5 ppm except in the contaminant plume area, where the oxygen concentrations have been consumed by aerobic biodegradation. The vertical exchange of oxygen with the unsaturated zone is assumed to be insignificant. The injected oxygen concentration is 8 ppm. The BIOPLUME II model assumes that injected water provides enough nutrients to support microbial growth in the aquifer.

Figure 4 illustrates the potential well locations considered by the optimization. Six downgradient wells can potentially extract contaminated groundwater at rates between 0 and 20 gpm. The upper and lower bounds of hydraulic head for the extraction wells are 30.5 and 24.4 m, respectively. The cleanup standard, C_{cl} , is 3 ppm for the entire study area.

Figure 4 also identifies monitoring wells (not subject to optimization) used to observe whether the plume is captured during a three-year remediation period. Because the system can inject potentially much water, additional monitoring wells are installed in

the Western boundary. This helps ensure that unacceptable plume spreading does not result. The maximum contaminant concentration allowed to reach monitoring wells, C_{ca} , is 1 ppm.

Table 2 lists cost coefficients used to estimate system costs. The injection coefficient is based on the nutrients, oxygen and pumping operation costs. The extraction cost coefficient considers cost of treating and pumping contaminated groundwater. Treatment includes air stripping and granular activated carbon. Injection and treatment facilities capital costs are based on their capacities.

APPLICATIONS AND RESULTS

Optimal In-situ Bioremediation System Design with Fixed Cost

The first stage management goal is to minimize total system cost which includes pumping/treatment, well installation, and facilities capital costs. Below we contrast abilities of SA ,GA and PRSA varieties to achieve this goal. In SA we use a threshold accepting function and Corana's neighborhood search [Corana et al., 1987] to reduce SA computation cost and extend its ability to deal with continuous variables. Our two GA formulations are based on the methodology of McKinney and Lin [1994], but include replacing binary code with Gray code and use of uniform crossover. Our GAs also extend tournament size of tournament selection from 2 to 4 to increase selection intensity [Blickle and Thiele, 1996] and to improve convergence. We implement segregated GA to refine the search in both feasible and infeasible regions. The parameter choice of GAs and PRSA is problem-dependent. After some test runs, we choose a population size 100 for optimizing system design with fixed cost and 200 for minimizing cost of time-varying pumping strategy. Crossover and mutation rates used for GAs and PRSA are 0.9 - 1.0 and 0.01 - 0.03, respectively.

We use six formulations to compare the three optimization algorithms. Because of the stochastic nature of these algorithms, we run each formulation twenty times using different random seeds. Table 3 lists maximum, minimum and average system costs of these runs for six formulations. Figure 5 illustrates the error bars of six formulations. The upper and lower caps indicate the average system cost plus or minus one standard deviation, respectively. The large standard deviation reflects that the optimization algorithm does not converge to the same optimal solution consistently.

PRSA2 (PRSA with Boltzmann trial and explicit well installation) designs the least-cost system ($188,600). It also has the lowest average system cost ($193,900) and the smallest standard deviation (Figure 5). GA2 and PRSA2 perform well because of explicit well installation coding. GA1 and PRSA1 using implicit well installation do not converge to optimal solutions. It is difficult for GA1 and PRSA1 to reduce well numbers because implicit well installation depends on whether or not pumping rates reach zero. SA1 shows that SA can converge to optimal solutions but is not as stable as PRSA (note the large standard deviation in Figure 5). Threshold accepting helps SA1 and PRSA3 converge to optimal solution using fewer simulations. For example, PRSA3 reduces average number of simulation by 43% compared with PRSA2, while still maintaining reasonably good solution quality (low average system cost and small standard deviation).

Figure 6 shows the convergence behavior of SA, GA and PRSA. It illustrates the change of system cost vs. number of BIOPLUME II simulations as the optimization algorithms progress. We compare the best results of six formulations (minimum system cost of six formulations) in Figure 6. PRSA1 and GA1 converge slowly because of implicit well installation. GA2 has the fastest convergence but additional simulations do not improve solution quality. PRSA2 uses uphill moves (Boltzmann trial) and explicit well installation to gradually converge to optimality. SA1 and PRSA3 employ threshold accepting to reject some expensive system designs without requiring simulation. This reduces total simulations and computation effort. Table 4 compares optimal systems designed by the different approaches. All three algorithms design similar systems. All use three or four injection wells and one extraction well. However, the PRSA yields the least cost strategy.

Time-varying Pumping Strategy

The second stage management goal is to minimize injection, extraction and treatment costs plus facility capital costs that are functions of the flow rates. Employing the four wells (U1, U2, U4 and E1) selected in the first stage optimization, we develop time-varying pumping strategy for a three-year remediation consisting of six half-year pumping periods. Figure 7 contrasts steady and time-varying pumping strategies. Optimal time-varying pumping reduces total injection and extraction volumes by 27 % and total injection and extraction cost by 31% when comparing with the optimal steady-

This illustrates that minimizing in-situ bioremediation system design while including fixed cost is sometimes more important than merely minimizing time-varying pumping cost.

CONCLUSIONS

We present a parallel recombinative simulated annealing (PRSA) model to optimize in-situ bioremediation system design. The new simulation/optimization model determines the pumping (extraction/injection) strategy that minimizes total system cost, reduces contaminant concentration to the cleanup standard, and prevents contaminant plume migration. To improve PRSA convergence and performance, we employ Gray code, uniform crossover, explicit well installation coding, threshold accepting function (TAF) and segregated genetic algorithm. Compared with Boltzmann trial, TAF reduces computation cost 43 % by rejecting expensive system design without requiring simulations.

PRSA minimizes total system cost (pumping/treatment, well installation and facility capital costs) better than SA and GA. An optimal time-varying pumping strategy requires 31 % less pumping costs than an optimal steady pumping strategy. Optimizing system design while including fixed costs more significantly impacts total system cost than merely minimizing pumping/treatment costs for the 3-year in-situ bioremediation project.

Parallel recombinative simulated annealing is a general-purpose optimization approach that has the good convergence of SA and the efficient parallelization of GAs.

Table 2. Cost function coefficients

Coefficients	Value
Discount rate	0.05
C^P for injection cost (oxygen, nutrient and pumping operation)	300 ($ per gpm-year)
C^P for extraction cost (treatment and pumping operation)	1,000 ($ per gpm-year)
C^{IP} (well installation cost)	12,000 ($ per well)
D (injection facility capital cost)	D_{20gpm} = \$ 20,000 D_{40gpm} = \$ 24,000 D_{60gpm} = \$ 28,000 D_{80gpm} = \$ 32,000 D_{100gpm} = \$ 36,000 D_{120gpm} = \$ 40,000 D_{140gpm} = \$ 44,000
E (treatment facility capital cost)	E_{20gpm} = \$ 30,000 E_{40gpm} = \$ 38,000 E_{60gpm} = \$ 46,000 E_{80gpm} = \$ 54,000 E_{100gpm} = \$ 62,000 E_{120gpm} = \$ 70,000

These two are probably not linear function but nonlinear functions of the flowrate.

Note : 1 gpm = 0.06309 liter/sec.

URGENT ! PLEASE RETURN REVIEW WITHIN FOUR WEEKS.

Water Resources Research's Manuscript Appraisal Form

A r: Dr. Richard C. Peralta **Reviewer #** 3

Title: Optimal in-situ bioremediation system design using parallel recombinative simulated annealing

MS # (WR97-605)

The following questions and comments are provided as a guideline for reviewers. Please provide additional detailed comments in a written report. This form and your written report will be forwarded unedited to the author. Avoid phrasing that might generate antagonism by exaggerated, cynical, or derogatory remarks. Any confidential remarks for the editors should be included in a cover letter. Note that the paper need not agree with currently popular opinions or with your own view in order to be publishable. To serve its readership well, it is important that *WRR* provide a forum for widely diverse scientific views.
Please use either black or blue ink pens. Avoid the use of red/blue pencils on this form as these marks do not photocopy well.

1. CONTRIBUTIONS AND AUDIENCE
   What are the important contributions of this paper?

2. TECHNICAL SOUNDNESS
   Is the paper technically sound? See Attached.

   Are the methods described fully?

   Is the mathematical development complete and accurate?

3. PRIOR PUBLICATION
   Has this work, or very similar work, been published elsewhere?

4. ORGANIZATION AND STYLE
   Is the paper well written and organized?

   Are all tables and figures necessary?

   Can the paper be shortened?

5. EVALUATION
   (a) Does this paper make a significant, new contribution in the area of water resources?

   (b) How do you rate the paper?

   Outstanding ____ Very Good ____ Good ___ Fair _X_ Poor ____

Review of "Optimal In-Situ Bioremediation System Design Using Parallel Recombinative Simulated Annealling" by Shieh and Peralta 3

The authors present an applied study that explores some influences of di rent stochastic optimization algorithms for solution of an opt.mal bioremediation design problem in an idealized hydrogeologic setting. They examine various implementations of simulated annealing, genetic algorithms, and a combination of the two. In its present form I would not consider the paper to stress any new theoretical development, and from this particular perspective I question that it is an appropriate manuscript for publication in WRR.

The paper contains some interesting results pertaining to solution methods for optimal groundwater management models. These may very well be appropriate for publication in a journal with a more applied focus. If the authors wish to publish their results in WRR, I suggest that the paper be shortened considerably, and made to focus on the numerical results and the particular encoding schemes used (less in terms of introductory material and the BioPlume II model, and more detail on novel mathematical representations). In this case the paper should be short enough to consider as a technical note rather than a full paper.

More generally, the authors should strive to bring out specific aspects of their experimental design and the results obtained, and to discuss them in appropriate detail. To often, the current paper tends to read as a brief review of many interesting pieces of information that, while related, do not seem to build on each other to produce a substantial new contribution to knowledge. This may, of course, be sir 'y the result of particular decisions by the authors about what ma. .ial to present in a limited amount of space.

A few more specific comments follow:

1. On page 4, "the new techniques are robust ..." In what sense are they robust? Robustness in this sense would be related to an ability to consistently find a local optimum, at least. Note that robustness would not be related to the ability to run to completion and produce some type of result, as important as that may be in a practical context.

2. On page 9, "traditional optimization techniques such as mixed integer nonlinear programming cannot apply to equation (1) which is not differentiable." Strictly speaking all binary or integer optimization problems are non-differentiable, and often involve some type of implicit enumeration solution method as a result (e.g., branch and bound). The classical linear fixed charge problem is an example of a non-differentiable cost function that is often addressed via binary variables, resulting in an IP, MILP, or MINLP. The authors may wish to rethink the specific reasons why they preferred to avoid these classical approaches.

3. I did not understand the difference between eqs. (3) and (4).

4. The description of explicit well coding on page 15, which the au ors have invented, is too sketchy to provide a full understanding of .ne approach.

5. On page 16, beginning of paragraph 3 ("This TAF..."), it is not clear at this point that the TAF replaces the Boltzman distribution.

6. The penalty terms and the segregation method could be interesting but it is not explained nor explored in sufficient detail. This may be one candidate to expand upon in a future version. For example, Step 5 is stated: "Exchange individual solutions between the new large penalty and small penalty parent populations."

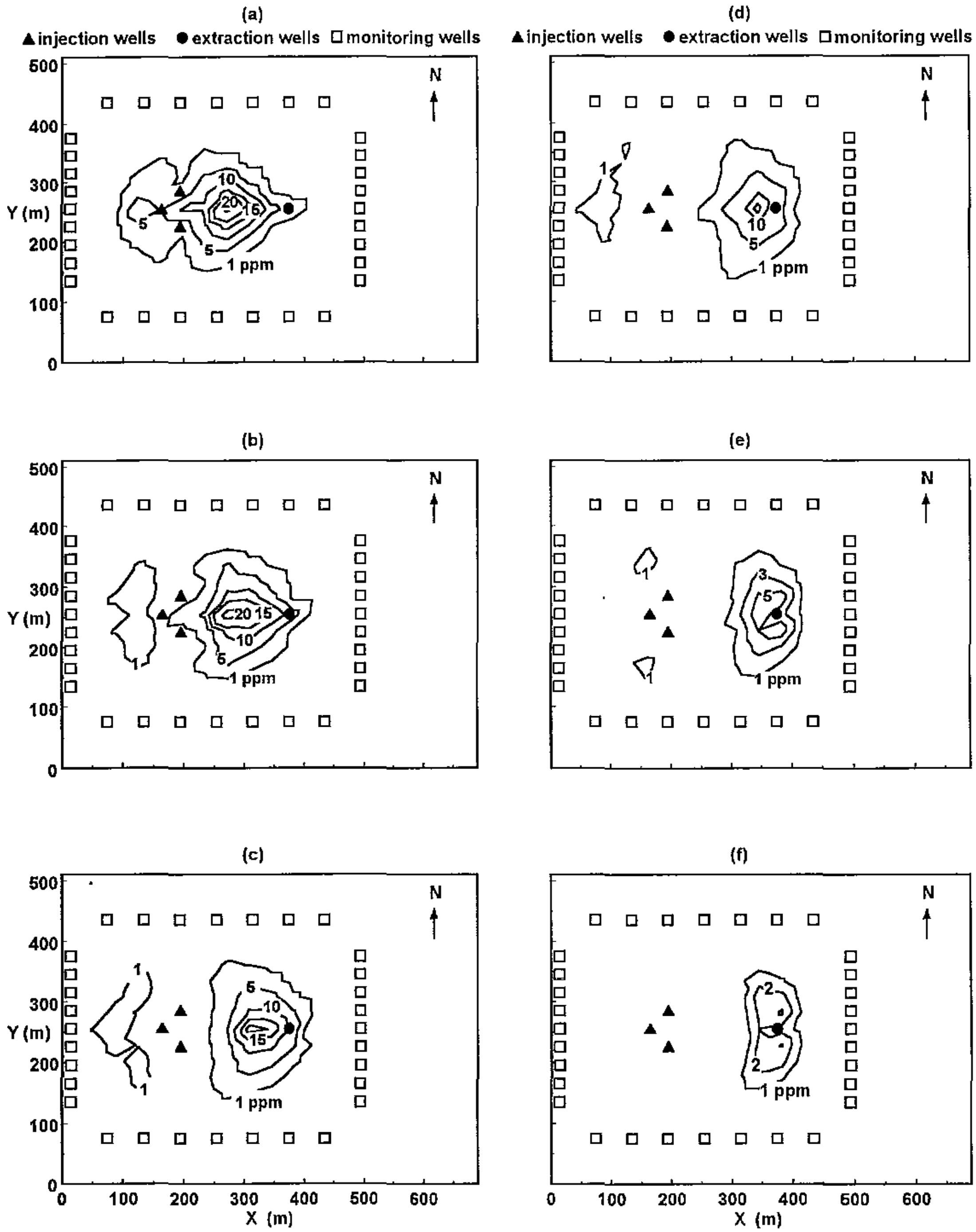

Figure 8. Change of contaminant plume using time-varying pumping strategy after in-situ bioremediation (a) 0.5 yrs, (b)1.0 yrs, (c) 1.5 yrs, (d) 2.0 yrs, (e) 2.5 yrs, and (e) 3.0 yrs