

ground water

Dynamic Optimal Ground Water Remediation Including Fixed and Operation Costs

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Abstract/

In time-varying ground water remediation, the lack of an optimal control algorithm to simultaneously consider fixed costs and time-varying operating costs makes it nearly impossible to obtain an optimal solution. This study presents a novel algorithm that integrates a genetic algorithm (GA) and constrained differential dynamic programming (CDDP) to solve this time-varying ground water remediation problem. A GA can easily incorporate the fixed costs associated with the installation of wells. However, using a GA to solve for time-varying policies would dramatically increase the computational resources required. Therefore, the CDDP is used to handle the subproblems associated with time-varying operating costs. A hypothetical case study that incorporates fixed and time-varying operating costs is presented to demonstrate the effectiveness of the proposed algorithm. Simulation results indicate that the fixed costs can significantly influence the number and locations of wells, and a notable total cost savings can be realized by applying the novel algorithm herein.

Introduction

The pump-and-treat method is one of the most common ground water remediation methods. The feasibility of coupling optimization techniques with ground water flow and transport simulation to design pump-and-treat systems has been extensively studied (Gorelick et al. 1984; Ahlfeld et al. 1988; Andricevic and Kitanidis 1990; Yeh 1992; Sawyer et al. 1995; McKinney and Lin 1995; Wang and Zheng 1998; Mansfield and Shoemaker 1999). Chang et al. (1992) employed an optimal control method, called the successive approximation linear quadratic regulator (SALQR), to design a time-varying pumping system for the remediation of contaminated aquifers. Culver and Shoemaker (1992) determined that time-varying policies are more cost effective than time-invariant policies. The SALQR algorithm has been shown to be efficient in solving time-varying problems (Mansfield et al. 1998; Yoon and Shoemaker 1999). Although superior in dealing with the time-varying problems, SALQR fails to cope with problems with fixed costs.

Pump-and-treat system design is important because well locations and pumping rates can markedly affect system performance. Generally, the decision variables involve determining the values of pumping rates from extraction wells and selecting the locations of wells. Owing to the discontinuous nature of well location selection, mathematical programming is often simplified by neglecting the fixed costs of well installation. The optimal network normally consists of those wells whose final, optimized pumping rates are nonzero. However, this simplification can lead to designs that rely on numerous wells pumping at small rates over long periods (McKinney and Lin 1995). Recently, researchers have investigated various methodologies for incorporating these fixed costs. McKinney and Lin (1994, 1995) employed a genetic algorithm (GA) and mixed-integer nonlinear programming (MINLP) to solve ground water management problems, including both fixed and operating costs; however, the authors assumed time-invariant pumping rates and steady-state conditions. Zheng and Wang (1999) integrated tabu search and linear programming to design optimal ground water remediation, by accounting for both fixed and operating costs, but, again, only time-invariant pumping rates were considered. Aly and Peralta (1999) used the L_{∞} norm as a global measure of aquifer contamination, rather than the traditional control locations for contaminant concentrations. They compared the performance of a GA with that of a MINLP. Rizzo and Dougherty (1996) solved a large-scale, six-management-period problem, using simulated annealing. Although the

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models by Aly and Peralta (1999) and Rizzo and Dougherty (1996) can be applied to a dynamic system with fixed and operating costs, these authors decoupled the problem into several period-wise subproblems, which they solved sequentially and independently. The approach is thus not one of fully dynamic optimization, and the results may not be the optimal solution of the originally defined problem. Huang and Mayer (1997) and Wang and Zheng (1997) used a GA to find the optimal pumping rates and the discrete fixed costs of well locations in dynamic ground water remediation management. Wang and Zheng (1998) applied a GA and simulated annealing, coupled with the MODFLOW finite difference ground water flow model, for optimal ground water remediation design over multiple management periods, and including both fixed and operating costs. Because a GA or simulated annealing alone cannot explore the stage-wise structure of the nonlinear dynamic operating cost, the major drawback of applying these combinatorial algorithms to solve the contaminated ground water problem is the dramatic increase in computational loading (Culver and Shoemaker 1997). Hence, their approach has only limited capability to determine dynamic pumping rates. The maximum number of planning periods considered by the previous three studies is only four. Watkins and McKinney (1998) applied a generalized Benders decomposition and outer approximation to solve an MINLP formulation of a conjunctively managed surface and ground water system, involving cost functions with both discrete and nonlinear terms. They applied the response matrix approach to develop constraints on their optimization problem. The response matrix method requires that the system transfer function be assumed as linear. The approach is not directly applicable to the remediation problem because a ground water remediation problem always has nonlinear transfer function (Gorelick et al. 1984).

Related investigations have demonstrated that dynamic policies are more cost-effective than the best static policies because pumping policies are allowed to change as the contaminant plume moves (Chang et al. 1992; Culver and Shoemaker 1992). Owing to dynamic optimal control algorithms requiring a separable objective function for each stage t , they face difficulties in solving a problem with an objective function that contains fixed costs. Culver and Shoemaker (1997) used quasi-Newton differential dynamic programming (QNDDP) for ground water reclamation with treatment capital. Culver and Shenk (1998) also employed QNDDP to solve a dynamic optimal pump-and-treat ground water remediation problem with an objective function that included the operating and capital costs of a granular activated carbon system. Culver et al. (1997) and Culver and Shenk (1998) assumed the capital cost of the system to be a continuous function of the pumping rate at the first time step. Accordingly, the summation of capital and operating costs is also a continuous objective function. The main difference between the work of Culver et al. (1997) and Culver and Shenk (1998) and this study is that their algorithm cannot be applied to a problem with a discrete objective function, such as the network design problem considered here. Sun and Yeh (1998) employed location and schedule optimization to design a ground water remediation system using a soil vapor extraction system. Although their model determines extraction well locations and the time-varying extraction schedule, their approach is essentially numerical and requires

the pumping rates to be discretized. The computational capability of their approach is limited for a dynamic system, because the computational loading increases significantly with the number of both conceivable pumping rates and planning periods.

While attempting to resolve the planning problem of simultaneously considering the fixed costs of well installation and the operating costs of time-varying pumping rates, previous studies have their computational limitations. The GA is attractive because it does not require the differentiability of the objective function. Hence, the GA can easily incorporate the fixed costs associated with the ground water remediation problem. However, applying this technique alone to solve time-varying policies would dramatically increase the computational resources required. Therefore, this study presents a novel approach for resolving this optimization problem by effectively combining a GA with constrained differential dynamic programming (CDDP).

However, system planning commonly assumes that an "optimal solution" is restricted and defined by its formulation, the objective function, and constraints, rather than being the best general solution. The next section defines "optimal ground water remediation." No optimization algorithms consider all phases of a real problem. An optimal solution is the beginning rather than the end of a decision-making process.

Formulation of the Management Model

The management model attempts to minimize the total cost of remediation, composed of the fixed costs of well installation and operating costs of the pumping and treatment system. The problem can be formulated as

$$\begin{aligned} & \min_{\substack{I \subset \Omega \\ u_t^i, i \in I, t = 1, \dots, N}} \\ J(I, u_t(I)) = & \sum_{i \in I} \left\{ a_1 y^i(I) + \sum_{t=1}^N \left[a_2 u_t^i(I) \right. \right. \\ & \left. \left. + a_3 u_t^i(I) (L_*^i(I) - h_{t+1}^i(I)) \right] \right\} \end{aligned} \quad (1)$$

subject to

$$\{x_{t+1}\} = T(x_t, u_t(I), t), \quad t = 1, 2, \dots, N, I \subset \Omega \quad (2)$$

$$c_{Nj} \leq c_{\max}, j \in \Phi \quad (3)$$

$$\sum_{i \in I} u_t^i \leq u_{\text{total}}, \quad t = 1, 2, \dots, N \quad (4)$$

$$u_{\min}^i \leq u_t^i(I) \leq u_{\max}^i, \quad t = 1, 2, \dots, N, I \subset \Omega, i \in I \quad (5)$$

where Ω is an index set that defines all candidate well locations in the aquifer; and I is a potential network alternative

(design) and a subset of Ω . The upper index i denotes a well in the network design (I). $J(\cdot)$ represents the total cost of I ; $x_t = [h_t; c_t]^T \in R^{(n_h+n_c) \times 1}$ is the state of continuous variables representing heads (h_t) and concentrations (c_t); and n_h and n_c denote the total number of hydraulic heads and concentrations, respectively; $u_t(I) \in R^{m \times 1}$ represents the vector of control variables whose dimension depends on I ; m is the number of control variables; $T(x_t, u_t(I), t)$ represents the transition equation; Φ is the set of observation wells; a_1 , a_2 , and a_3 are factors used to convert the well installation cost, treatment cost, and operating cost, respectively, into monetary values; $L_g(I) \in R^{m \times 1}$ is the distance from the ground surface to the lower datum of the aquifer for wells; $h_{t+1}(I)$ denotes hydraulic head for nodes at time $t + 1$; $y(I)$ is the depth of wells; and u_{total} represents the maximum allowable total pumping rates from all extraction wells. Equation 5 specifies the capacity constraints for each well. The transition equation, T , in Equation 2 is solved with ISOQUAD (Pinder 1978), a finite-element ground water flow and transport model for a confined two-dimensional aquifer. The transport model includes changes in head caused by pumping and changes in the contaminant concentration owing to advection, diffusion, dispersion, and linear equilibrium sorption. In practical applications, the set of observation wells (Φ) is the group of sites that are made to meet the water-quality standard, and N is the time limit within which the standard must be met. Certain well locations can easily be excluded from consideration by excluding the well sites from the Ω set that is defined by the user.

The total cost objective function in Equation 1 is mixed-integer nonlinear. Therefore, the ground water remediation model defined by Equations 1 through 5 is a mixed-integer time-varying optimization problem. The first component in Equation 1 is the costs of well installation, and is incurred if a well is installed for pumping. The costs of well installation are a discrete operation and required the use of binary variables in the optimization model. The second component in Equation 1 is the operating cost, involving pumping and treatment costs. These costs are continuous functions of the state and control variables and are separable functions for each stage t . Because of the discrete nature of the installation cost, the problem, defined by Equations 1 through 5, is difficult to solve using CDDP alone (Chang et al. 1992; Culver and Shoemaker 1992). Meanwhile, the near global optimization techniques, such as simulated annealing (Rizzo and Dougherty 1996), a GA (Huang and Mayer 1997), or tabu search (Zheng and Wang 1999), do not require the objective function to be continuous, convex, or differentiable. Hence, these techniques are potentially capable of solving an optimization problem containing fixed costs. However, applying these techniques to solve time-varying policies would dramatically increase the computational resources required (Culver and Shoemaker 1997; Zheng and Wang 1999). Therefore, the techniques mentioned are inappropriate for time-varying optimization.

Integration of a GA and CDDP

This investigation integrates a GA and CDDP (GCDDP) to solve the problem defined by Equations 1

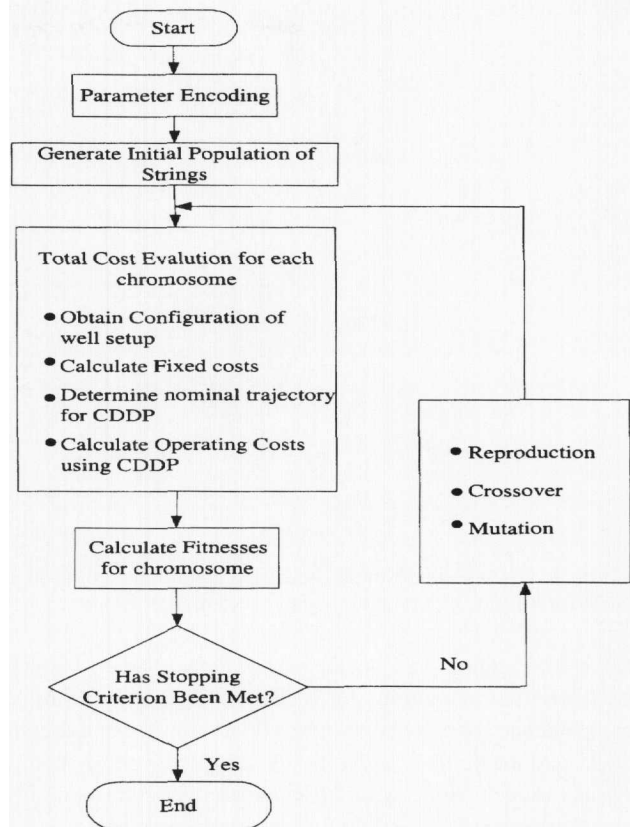


Figure 1. Flowchart for the ground water remediation model.

through 5. In this integrated approach, the GA, a near global optimization algorithm, is used to locate the optimal well sites, whereas CDDP is employed to calculate the optimal pumping rates. Figure 1 illustrates the procedure of the algorithm. According to this figure, the algorithm is a simple GA with CDDP embedded to compute the optimal operation costs for a potential network alternative (represented by a chromosome). The total cost for each network alternative (chromosome) is the sum of the optimal operation costs and its fixed costs. In this investigation, time-varying pumping rates are considered while evaluating the optimal operation costs using CDDP. These procedures are clarified by the following step-by-step procedure.

Step 0: Initialization

Encode the network alternatives as chromosomes and randomly generate an initial population. GA is widely known to use binary coding to represent a variable. This study uses a binary indicator to represent the status of the wells installation on a candidate site. Thus a chromosome, represented by a binary string, defines a network alternative. Each bit in a chromosome is associated with a candidate site, and the length of the chromosome is equal to the total number of candidate sites available for well installation. If the value of a bit is equal to one, the associated candidate site will install a well; otherwise, the value of a bit equals zero, and the associated candidate site will not install a well.

To demonstrate the operation of chromosome encoding, a hypothetical, homogeneous, isotropic confined aquifer with dimensions of 600 m \times 1200 m serves as an

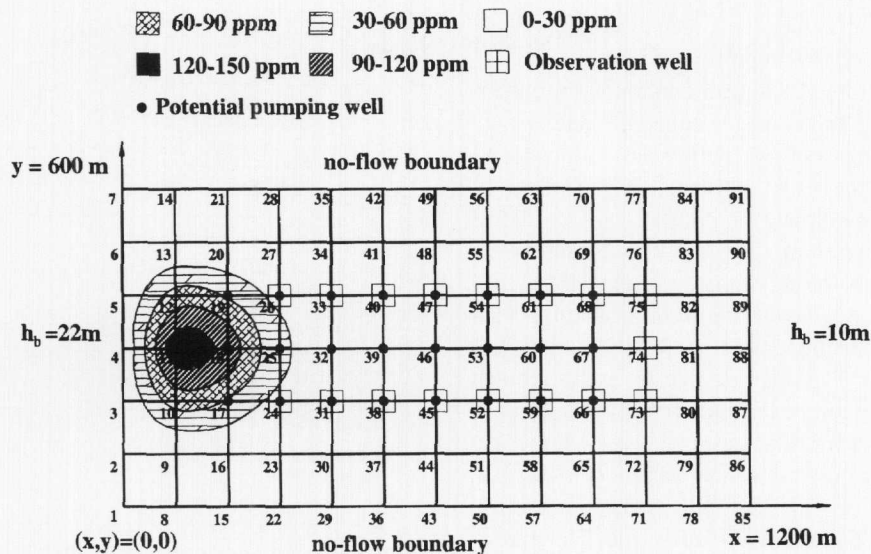


Figure 2. Finite-element mesh, boundary conditions, initial plume, and locations of numbered observation and potential extraction wells for all runs of the ground water reclamation example.

example. Figure 2 presents the finite-element mesh, associated boundary conditions for hydraulic head and contaminant concentration, location of candidate sites for extraction wells, and location of observation wells. There are 91 finite-element nodes, along with 24 candidate well sites, and 17 observation wells.

Because the hydraulic head, initial concentration, locations of observation wells, and candidate sites for pumping wells, are symmetrical in Figure 2, this study assumes that the optimal network is also symmetrical. According to this assumption, the combination of network configurations will decrease in a GA and the computational effort will reduce. The chromosome contains 16 bits, where the first eight bits represent the sites along the centerline and the last eight bits represent candidate sites in the upper region. When a bit among the last eight bits has a value, it represents two wells placed symmetrically to the centerline. Because the well selection is binary, encoding and decoding the chromosome is straightforward.

Step 1: Evaluate the Total Cost and Fitness of Each Chromosome.

In this investigation, the fitness equals the reciprocal of total cost. The chromosome that was described in Step 0 can be represented as a binary string in the form $I_1 = i_1, i_2, \dots, i_8, i_9, \dots, i_{16}$, where I_1 denotes a chromosome within the population. Each digit i_e has a value of either 1 or 0. The number of wells for the chromosome can be calculated as

$$q_{\text{well}_1} = \sum_{e=1}^8 i_e + 2 \sum_{e=9}^{16} i_e \quad (6)$$

The total cost for each chromosome, or network alternative, includes the fixed and associated operating costs. The fixed cost in Equation 1 can be evaluated before optimal operating costs are calculated because each chromosome defines the number and location of pumping wells in

the network design. For each chromosome, an embedded CDDP algorithm is then applied to determine the optimal operating cost.

According to Equations 1 through 5, when a network alternative is selected, the discrete and inseparable nature of the problem is eliminated. The optimization model for each chromosome can then be rewritten as

$$\min_{u_i^i, i \in I, t=1, \dots, T} J(I, u_t(I)) = \sum_{i \in I} \left\{ \sum_{t=1}^N \{a_2 u_t^i(I) + a_3 u_t^i [L_*^i(I) - h_{t+1}^i(I)]\} \right\} + c_{\text{fix}} \quad (7)$$

subject to

$$\text{Equations 2, 3, 4, and 5} \quad (8)$$

where I represents a chromosome, and C_{fix} is a constant that represents the fixed costs for the chromosome. C_{fix} is a constant and, therefore, does not influence the determination of the operating costs. Hence, for each chromosome, Equations 7 and 8 define a standard dynamic optimal control problem that can be solved by CDDP. The total cost for each chromosome is calculated after the optimal operating cost is determined using CDDP. Selection, crossover, and mutation can generate the next improved generation of chromosomes after the total costs for all the chromosomes in a generation are determined.

The CDDP used herein is a modification of SALQR (Chang et al. 1992). Using a penalty function to incorporate the water quality and extraction constraints (Equations 3 through 5 into Equation 7), SALQR solves the optimization problem as an unconstrained problem. This study uses the penalty function to resolve the water quality constraints (Equation 3) and applies quadratic programming at each stage in the backward and forward sweep of CDDP algorithm to handle the control constraints in Equations 4 and 5 (Murray and Yakowitz 1979). The penalty function used in this study has the following form (Lin 1990):

Table 1
Aquifer Properties of the Example Application

Parameter	Value
Hydraulic conductivity	4.31×10^{-4} m/sec
Longitudinal dispersivity	70 m
Transverse dispersivity	3 m
Diffusion coefficient	1×10^{-7} m ² /sec
Storage coefficient	0.001
Porosity	0.2
Sorption partitioning coefficient	0.245 cm ³ /g
Media bulk density	2.12 g/cm ³
Aquifer thickness, b	10 m
L_s	120 m

$$P_k(f_k) = \xi_k \quad \xi_k \leq 1 \quad (9)$$

$$P_k(f_k) = c_1 \xi_k^2 + c_2 \xi_k^{1/2} + c_3 \quad (10)$$

with

$$\xi_k = (w_k^2 f_k^2 + \epsilon_k^2)^{1/2} + w_k f_k \quad (11)$$

where w_k is the weighting coefficient of the k th constraint, ϵ_k is a shape parameter of the hyperbolic function ξ_k , and c_1 , c_2 , and c_3 are constant coefficients. Chang et al. (1992) demonstrated that this hyperbolic penalty function, ξ_k , is numerically efficient; Culver and Shoemaker (1992, 1993, 1997), as well as Mansfield and Shoemaker (1999) later used it. In all cases, weights on the penalty function increased until an optimal solution that did not significantly violate the constraints was found. Each CDDP calculation requires an initial nominal policy to start. This study uses a "do nothing" policy (all zero pumping rates) as an initial nominal policy for all the chromosomes.

Step 2: Reproduce the Best Strings

The GA selects parents from a population of strings (chromosomes) based on the fitness associated with each string. This study carries out reproduction by tournament selection (Wang and Zheng 1997). The selection mechanism plays a prominent role in driving the search toward superior individuals and maintaining high genotypic diversity in the population. In each tournament selection, a group of individuals is randomly chosen from the population, and the fittest individual is selected for reproduction. The procedure is repeated until the number of chromosomes required for crossover is fulfilled.

Step 3: Perform Crossover

Crossover involves randomly coupling the newly reproduced strings, with each pair of strings partially exchanging information. Crossover aims to exchange gene information to produce new offspring strings that preserve the best material from both parent strings. Generally, the crossover is performed with a certain probability (p_{cross}) to ensure that it is performed on most of the population. Herein, one point crossover is selected.

Table 2
Sensitivity Analysis on the Parameters
for the Case of \$120/m Unit Fixed Cost

P_{cross}	0.5	0.6	0.7	0.8
Population	O.V.	O.V.	O.V.	O.V.
60	90.10	89.49	89.49	90.10
70	89.49	90.20	89.49	90.10
80	96.26	90.10	89.49	90.10
90	90.10	89.49	90.10	89.49

P_{cross} = crossover probability.
Population = population size.
O.V. = The optimal value of objective function (divided by 1000).

Step 4: Implement the Mutation

Mutation restores lost or unexplored genetic material to the population, preventing the GA from prematurely converging to a local minimum. A mutation probability (p_{mutat}) is specified so that random mutations can be applied to individual genes. DeJong (1975) originally suggested that a mutation probability inversely proportional to the population size would prevent the search from locking onto a local optimum. This study follows DeJong's suggestion. Before implementing a mutation, a random number with uniform distribution is generated. If this number is smaller than the mutation probability, then mutation is performed; otherwise, mutation is disregarded. Notably, according to the specific probability, mutation changes a specific gene (0→1 or 1→0) in the offspring strings produced by the crossover operation.

Step 5: Perform Termination

After completion of Steps 1 to 4, a new population is formed. The new population requires evaluating the total cost as in Step 1, which is used to assess the stopping criterion. The stopping criterion is based on the change of either objective function value (total cost) or optimized parameters. If the user defined stopping criterion is satisfied or when the maximum allowed number of generations is achieved, the procedure terminates; otherwise, return to Step 1 to perform another cycle. The success and performance of the GA depend on several parameters: population size, number of generations, and the probabilities of crossover and mutation (McKinney and Lin 1994). Goldberg (1989) has suggested that a good GA performance requires the choice high-crossover and low-mutation probabilities and a moderate population size. Therefore, the GA does not generally guarantee optimality. However, GAs are robust and easy to hybrid with other optimization methods or simulation models.

Numerical Results

A ground water reclamation test problem, which is a modification of the example from Chang et al. (1992) and Culver and Shoemaker (1993, 1997), is adopted to verify the effectiveness of the methodology discussed in the preceding section. Figure 2 displays the aquifer. The hydraulic head distribution prior to pumping is assumed to be steady, the initial peak concentration within the aquifer is 150

Table 3
The Values of the Cost Function Coefficient
in the Example Problem

Coefficient	Value
a_1	\$0/m to \$240/m
a_2	\$40,000/(m ³ /sec·simulation period)
a_3	\$1000/(m ³ /sec·m·simulation period)

mg/L, and the water quality goal at the end of five years must be < 0.5 mg/L (c_{max}) at all the observation wells. The time between each stage in the management model is 91.25 days. Table 1 lists the properties of the aquifer. The performance of all examples relies on proper setting of the crossover probability (p_{cross}), population size, and mutation probability (p_{mutat}). Numerical experiments with a unit fixed cost (a_1) that equals \$120/m are performed for sensitivity analysis. This is then applied to the GA's parameters with p_{cross} that ranges from 0.5 to 0.8, and a population size, which ranges between 60 and 90, and $p_{mutat} = 1/\text{population}$ (adapted from DeJong's 1975 suggestion). Table 2 presents experimental results, which indicates that within the selected range the parameters affect the optimal values only slightly. Although the sensitivity analysis is applied to the case with the unit fixed cost equal to \$120/m, the problem's structure is similar for cases with other unit fixed costs. Therefore, the following examples are solved with $p_{cross} = 0.7$ and population size = 70, based on the results of the sensitivity analysis.

Cases with Uniform Unit Fixed Costs

This case contains 24 potential installation sites for pumping wells that remove the contaminant plume (Figure 2). The optimization problem determines a network design, which includes the number and locations of wells as well as pumping scheme, to remove the plume with minimum total cost. As stated in the Introduction, mathematical programming often neglects the fixed cost of well installation because of its discontinuous nature. The optimal network normally contains wells that have final, optimized nonzero pumping rates. However, the simplification can facilitate designs that rely on numerous wells that pump at small rates over long periods (McKinney and Lin 1995). This example was used to demonstrate that the network design problem with fixed costs could be resolved via GCDDP. In this situation, the number and locations of pumping wells as well as the pumping rates for each well are all decision variables. Table 3 displays the value of the cost-related coefficients, a_1 , a_2 , and a_3 . Table 4 summarizes the solutions of this case. As presented in Table 4, when the fixed unit cost increased from \$0/m to \$240/m, the number of wells decreased and the operating cost increased. For no fixed cost, the optimal design requires seven wells, whereas when the unit fixed cost is \$240/m, only one well is required. For no fixed cost and a fixed cost of \$240/m, the minimum total pumping volume among the wells is only 4.37 (L/s·simulation period) and 502.59 (L/s·simulation

Table 4
Optimal Solutions and CPU Time for the
GCDDP with Uniform Unit Fixed Costs

Fixed Unit Costs	\$0/m	\$60/m	\$120/m	\$240/m
No. of well	7	2	2	1
Total operating cost (\$)	56,341	60,690	59,909	75,690
Total cost (\$)	56,341	75,090	88,709	104,490
Minimum total pumping volume (L/sec·simulation period)	4.37	74.27	179.15	502.59
Number of generation	21	23	33	16
CPU time with bookkeeping method (second)	36,918	42,825	53,606	37,460
CPU time without bookkeeping method (second)	238,051	152,423	196,461	135,198

Runs are on a PC with AMD Athlon™ 1000 MHZ CPU.

Table 5
Total Cost Comparison With/Without Unit
Fixed Costs in GCDDP Optimization Model

Coefficient a_1	\$120/m	\$240/m
Total cost for the network designed without fixed costs (J_1)	157,141 (7 wells)	257,941 (7 wells)
Total cost for the networks designed with fixed costs (J_2)	88,709 (2 wells)	104,490 (1 well)
Ratio of difference ($(J_1 - J_2)/J_2$)%	77.14%	146.84%

period), respectively. This confirmed that if fixed cost is not considered, an optimal design tends to have several wells that pump at small rates. Table 4 also lists the CPU time and generation requirements of these cases. These cases were implemented on a PC with AMD Athlon™ 1000 MHZ CPU.

Figure 3 depicts the optimal network design and pollutant concentration distribution for the final planning period. Notably, all the concentration distributions are very similar to each other and satisfy the specified water quality standard at the observation wells shown in Figure 2. As the contaminant diffuses from west to east, pumping wells, which are located within the western region, are better equipped to remove the contaminant. In addition, the hydraulic head of the western region is higher than that of the eastern region. Therefore, the former pumping well requires less in pumping costs. Owing to these two reasons, pumping wells that have uniform unit fixed costs (Figure 3) are more likely to be situated in the western region.

Table 5 presents a comparison of the total network design costs of both fixed and no fixed cost. Within the comparison, the total cost design with no fixed costs was estimated by adding the operating costs to the fixed costs, which were estimated by multiplying the well depth by the unit fixed cost. Because the number of wells is unchanged, this total cost remains constant. Alternately, the total costs as well as number of wells in the designs with fixed costs varied according to the unit fixed cost. Table 5 displays that when the value of coefficient a_1 is \$240/m, the total

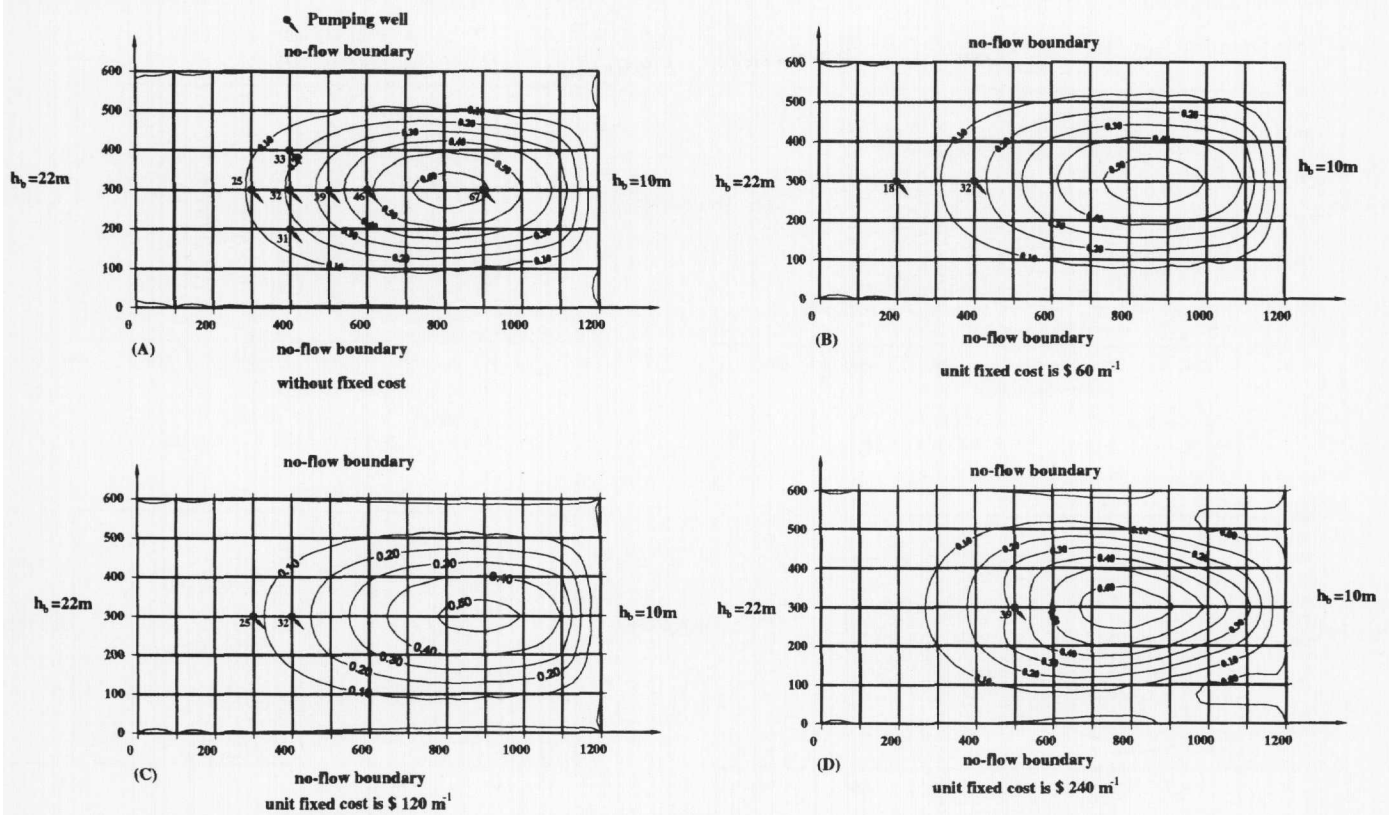


Figure 3. The optimal number of wells and concentration distribution by GCDDP at the end of five years.

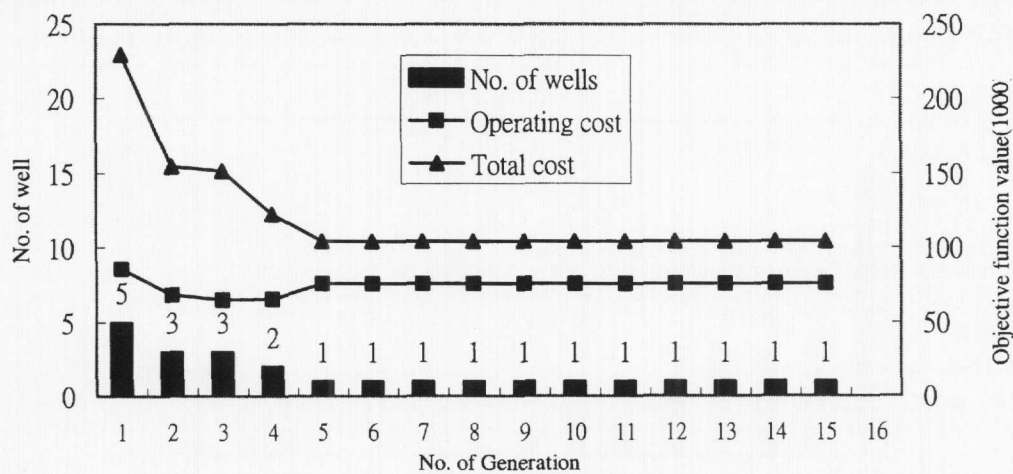


Figure 4. The objective function values and the number of wells versus the number of generations for the case of $a_1 = \$240/m$.

cost of the no fixed cost design exceeds the one with fixed costs by 146.84%. Therefore, designing a remediation network using an algorithm that considers fixed cost is important.

The GCDDP computation generates one superlative design (chromosome) among the population (70 chromosomes in this study) for each generation, and the best design is improved from generation to generation. Figure 4 demonstrates the evolution of the best design versus generation for the case of $a_1 = \$240/m$. Figure 4 also illustrates the change in the objective function value and the number of wells for the best chromosome of each generation. Although the operating costs increase at the fifth generation, the total costs always decrease in each generation and the solutions converge after the fifth generation.

Cases with Varying Unit Fixed Cost, a_1 , According to the Geological Conditions

Previously, both the unit fixed cost (a_1) and hydraulic conductivity were assumed to remain constant. However, because of geological heterogeneity, this is unlikely in reality. That is, the unit fixed cost (a_1) should vary according to the geological condition, and the optimal locations and well numbers will differ from that, which assumes a uniform unit fixed cost. A series of numerical examples was performed to examine the geological effects. Figure 5 depicts that the hypothetical examples consist of two distinct geological zones in which the unit fixed costs (a_1) vary among $\$0/m$, $\$60/m$, and $\$240/m$. The hydraulic conductivity is 1.29×10^{-4} m/sec. in Zone I and 8.62×10^{-5} in Zone II. Figure 5 also presents the optimal concentration distribution at the end of planning period and the optimal well

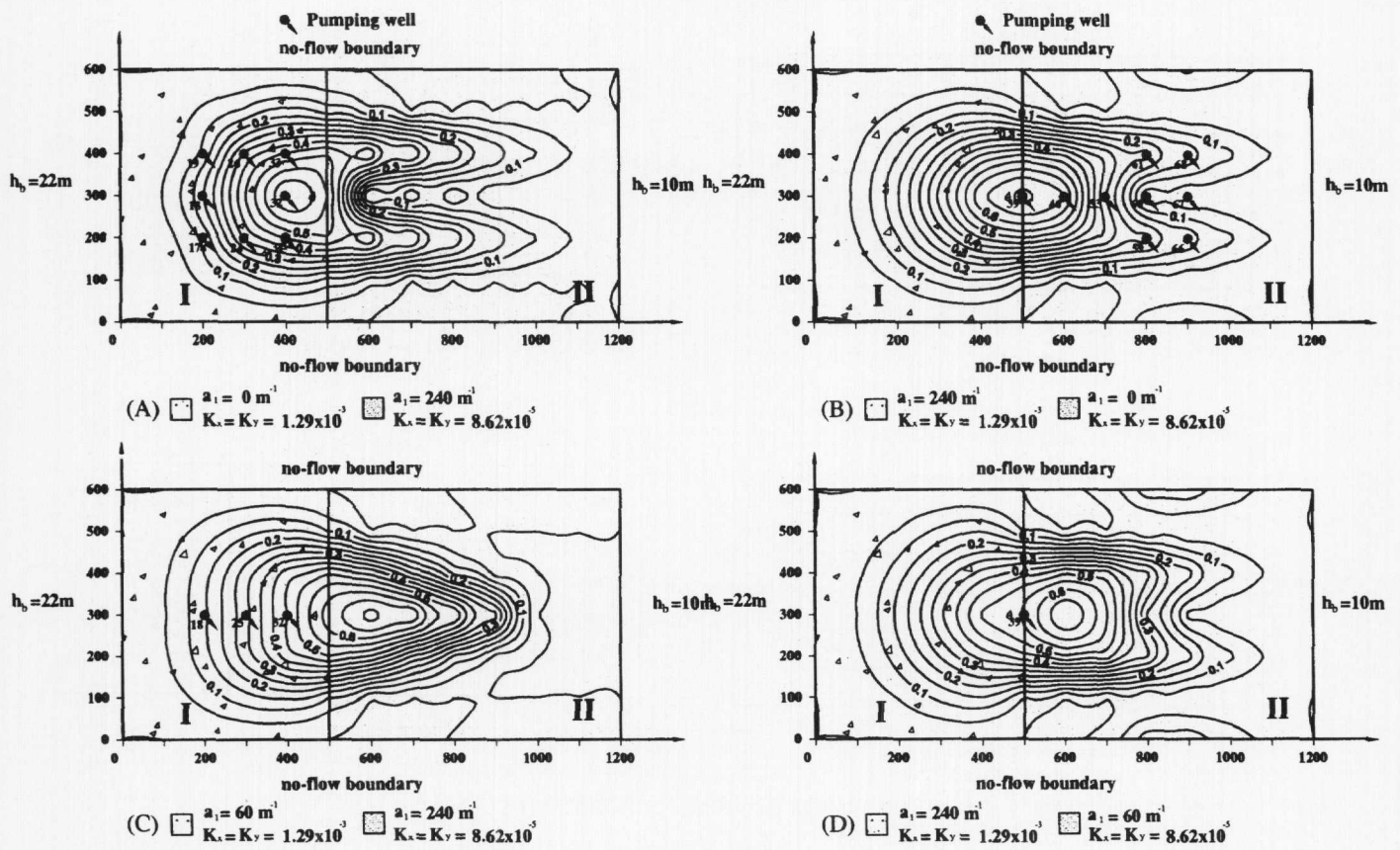


Figure 5. Optimal number of wells and concentration distribution at the end of five years for the varying fixed cost units.

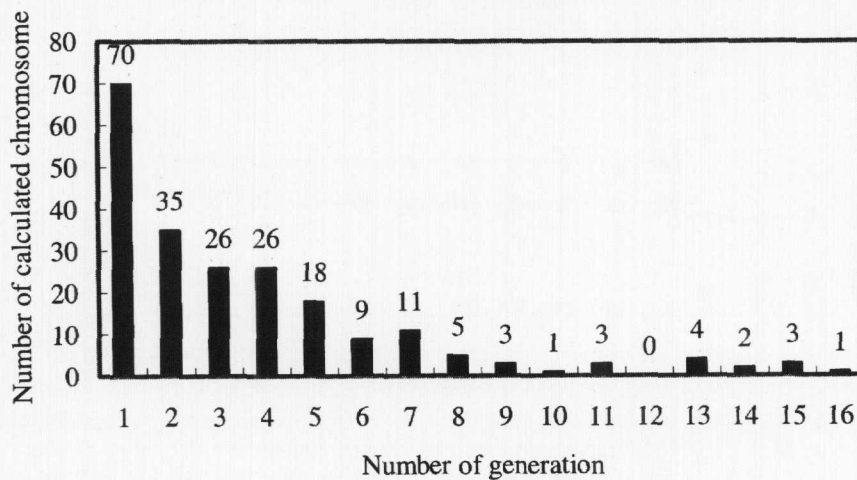


Figure 6. Calculated chromosome through 16 generations for case with unit fixed cost equaling \$240/m by the "bookkeeping" method.

number and location. All the concentrations satisfied the constraint (0.5 mg/L) at the observation wells. As described previously, when the unit fixed cost is uniform, the pumping wells are likely to be located on the upstream (the western region) of the aquifer because of initial concentration distribution and boundary hydraulic head condition. Nevertheless, when the unit fixed cost (a_1) varies based on geological conditions, pumping well distribution also varies (Figure 5). Figure 5a displays that, because a well costs less in Zone I than in Zone II, most wells are located in Zone I. Conversely, the pumping wells are concentrated in Zone II, where well installation costs are less (Figure 5b). When the fixed cost of zero (Figures 5a and 5b) increased to \$60/m (Figures 5c and 5d), well distribution in Figures 5c and 5d

is similar to that of Figures 5a and 5b; however, the number of wells is reduced in the former set because of a fixed cost increase. This demonstrates that the number and locations of wells vary according to the value and spatial pattern of the fixed cost, which depend on the geological conditions. Revealing this phenomenon via a conventional network design procedure, which ignores the fixed cost, is difficult. Accordingly, the proposed GCDDP algorithm provides a design that is nearer the true optimal solution than that of conventional algorithms.

Other Computational Issues

Considering the complexity of the proposed remediation problem, the programming efforts required to imple-

ment particular programming techniques to increase computational efficiency are not surprising. There are three methods to accelerate the computation, two of which have been implemented herein. The first one is to increase the computational efficiency of CDDP algorithm. Because each chromosome in the GCDDP algorithm requires a CDDP computation, accelerating the CDDP algorithm will reduce the computational time of the GCDDP algorithm significantly. The computing time of CDDP is reduced herein by exploring the sparse structure of the state derivative matrices of transition function ($\partial T/\partial x_i$) (Mansfield et al. 1998). Table 6 displays results with/without employing the sparsity in computation, which indicates that the CPU times are reduced roughly 7% of an algorithm that neglects it.

The second method is "bookkeeping." This method is to reduce the number of chromosome that must be evaluated by CDDP algorithm. As stated previously, a network design (a chromosome) is a subset of all candidate sites. Because the number of candidate sites is limited, the number of the subset (the chromosome) is countable and finite. Therefore, a chromosome with high fitness may likely repeat itself from generation to generation in the GA computation. Hence, a bookkeeping procedure records all chromosomes that the CDDP algorithm has evaluated. Within each GCDDP algorithm generation, a new chromosome is compared to previously recorded ones. If the chromosome already exists, a CDDP computation is not required and the algorithm proceeds to the next chromosome. The case with unit fixed costs of \$240/m is employed to illustrate the efficiency of this method. Notably, this case converges after 16 generations. The total number of required chromosomes is 1120; however, the CDDP algorithm calculates only 217 distinct chromosomes. Therefore, in this case, the bookkeeping method saves roughly 79% of chromosomes that require calculated by CDDP algorithm. Table 4 also gives the CPU time required for CDDP with/without the bookkeeping method. The table shows that the bookkeeping method can save significant CPU time. Figure 6 depicts the number of calculated chromosomes within the 16 generations. Figure 6 confirms that the number of calculated chromosomes decrease rapidly and saves significantly CPU resources. Owing to the high efficiency of chromosome encoding, each well requires only a single bit, and the additional memory that is required to implement the bookkeeping is minor.

The third method, which increases computational capability, is parallel computation. The GA is known to be easy and highly efficient for parallelism, which confirms its superiority over other combinatorial algorithms when resolving a ground water remediation design problem, such as simulation annealing and tabu search. Although this work does not review parallel computing the proposed model can be parallelized. Within the GCDDP algorithm, nearly 98% of CPU time is expended on chromosome evaluation (CDDP computing), which would benefit parallel computing because each chromosome is computed independently. Therefore, parallel computing can potentially increase the computational capacity of the GCDDP algorithm significantly and resolve large-scale problems.

Although GAs is a heuristic algorithm and provides no guarantee to converge on the global optimum, this does not

Coefficient a_1	CPU Time Per Iteration, (s)		
	\$0/m (7 wells)	\$120/m (2 wells)	\$240/m (1 well)
With employing the sparsity (T_1)	2.69	2.44	2.32
Without employing the sparsity (T_2)	2.88	2.66	2.47
Ratio of difference ($(T_1 - T_2)/T_2$)%	6.60%	8.27%	6.07%
Runs are performed on a PC with AMD Athlon® 1000 MHZ CPU.			

affect its usage (Goldberg 1989). The proposed GCDDP model is essentially also a heuristic algorithm. However, because the defined remediation problem is a discrete nonlinear and nonconvex one, no algorithms exist which can resolve it effectively. The proposed GCDDP model is the only algorithm that can provide a reasonable and valuable solution.

Conclusion

A GCDDP (an integration of a GA to CDDP) ground water remediation-planning model was developed to minimize the total cost of a pump-and-treat aquifer remediation system. Although the total cost including the fixed and operating costs should be included in the objective function of a ground water remediation problem, previous studies have never proposed an efficient algorithm to resolve this problem, owing to its combinatorial and dynamic characteristics. The proposed GCDDP algorithm calculates the minimum total cost while simultaneously considering the fixed and time-varying operating costs. A numerical study based on a homogeneous, isotropic confined aquifer revealed several prominent results.

When omitting the fixed costs in the optimization model, the GCDDP algorithm consistently designs a remediation plan with many wells pumping at small rates. On the contrary, the fixed costs considered can reduce the number and influence the locations of wells in the network design. Therefore, the total cost of GCDDP design can save significantly when the fixed costs are considered. In addition, this numerical study also demonstrates that the number and locations of wells may vary according to geological conditions. This phenomenon is difficult to reveal via a conventional network design procedure, which ignores fixed cost. Although the computational burden increased, this work increases the computation efficiency of the proposed GCDDP algorithm by exploring the sparse structure of the state derivative matrices of transition function and applying a bookkeeping programming procedure. Thus, the GCDDP algorithm is a feasible ground water remediation planning method. In summary, the novel GCDDP algorithm considers fixed cost, which is a significant factor of ground water remediation planning, to provide a more realistic solution. Parallel computation can further enhance the computational capacity of GCDDP to solve large-scale problems, which is receiving subsequent examination.

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